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1 **Factors controlling soil structure dynamics and carbon sequestration across different**  
2 **climatic and lithological conditions**

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15 **Abstract**

16 Soil organic carbon (SOC) is a strong determinant of soil fertility through its positive effects on soil  
17 structure and soil chemical and biological properties which in turn stimulate primary production. The  
18 objective of this work was to simulate field sites that represent different land uses and management  
19 practices in three continents, in order to identify the most important factors controlling soil structure  
20 dynamics and C sequestration across different climatic and lithological conditions as well as to  
21 quantify the rates of the afore-mentioned processes. The Carbon, Aggregation and Structure Turnover  
22 (CAST) model was used to simulate SOC sequestration, aggregate formation, and structure dynamics  
23 in three field sites including non tilled soils of natural ecosystems and tilled soils of agricultural fields  
24 in Europe (Critical Zone Observatories (CZO) of the SoilTrEC network) and one site in North  
25 America. Derived data from the simulations results, of SOC stocks and Water Stable Aggregate  
26 (WSA) particle size distribution, together with the respective results of three additional sites (Damma  
27 Glacier CZO, Milia (Greece) and Heilongjiang Mollisols (China)) were statistically analyzed in order  
28 to determine the factors affecting SOC sequestration and soil structure development. The natural

29 ecosystems include non tilled soils covered with natural local vegetation while the agricultural sites  
30 include cultivated and tilled soils covered with crops. The natural ecosystems were represented by  
31 Damma Glacier CZO (Switzerland), Heilongjiang Mollisols (China), Koiliaris CZO (Greece), Clear  
32 Creek (USA) and the Slavkov Forrest CZO (Czech Republic) whereas the agricultural field sites were  
33 located at Heilongjiang Mollisols (China), Koiliaris CZO (Greece), Clear Creek (USA), Marchfeld  
34 CZO (Austria) and Milia (Greece). Principal Component Analysis (PCA) identified clay content, bulk  
35 density, climatic conditions (precipitation and evapotranspiration), organic matter (OM) and its  
36 decomposition rates, as the most important factors that controlled soil structure development. The  
37 relative importance of each of these factors differs under differing climatic and lithological conditions  
38 and differing stages of soil development. Overall, the modeling results for both natural ecosystems  
39 and agricultural fields were consistent with the field data. The model reliably simulated C and soil  
40 structure dynamics in various land uses, climatic conditions and soil properties providing support for  
41 the underlying conceptual and mathematical modeling and evidence that the CAST model is a reliable  
42 tool to interpret soil structure formation processes and to aid the design of sustainable soil  
43 management practices.

44 Keywords: CAST model, soil structure, soil carbon, modeling

## 45 **1. Introduction**

### 46 **1.1 Soil threats**

47 The adoption of intense agricultural management practices, deforestation and livestock grazing has  
48 accelerated soil losses exceeding those of formation by approximately two orders of magnitude  
49 (Brantley et al., 2007) with important consequences for the role of soil in vegetation productivity  
50 worldwide (CEC, 2006). The EU as part of the 2006 Environment Policy Review previously  
51 published the Thematic Strategy for Soil Protection (CEC, 2006) as one of 7 thematic priorities. On 1  
52 January 2016, the 17 Sustainable Development Goals (SDGs) of the 2030 Agenda for Sustainable  
53 Development, adopted by world leaders in September 2015, officially came into force. One of the “17  
54 Goals to transform our World” by the United Nations, aims to protect, restore and promote sustainable

55 use of terrestrial ecosystems, sustainably manage forests, combat desertification, and halt and reverse  
56 land degradation and halt biodiversity loss (General Assembly, United Nations, 2015). Forests  
57 provide shelter to more than 80 per cent of all terrestrial species, 2.6 billion people depend directly on  
58 agriculture while 12 million hectares are lost every year due to drought and desertification, where 20  
59 million tons of grain could have been grown. Over 80 per cent of the human diet is provided by plants  
60 and 60 per cent of the energy intake is provided only by three cereals. As a result 74 per cent of the  
61 poor are directly affected by land degradation (General Assembly, United Nations, 2015). Despite its  
62 critical role in the sustenance of the biosphere and meeting the food requirements of more than 7  
63 billion global inhabitants, our knowledge of the soil functions and their response to human activity is  
64 far from complete. Thus, a great challenge in the soil science is to improve our understanding of soil  
65 processes, particularly for the critical soil functions as they are defined by EU Soil Thematic Strategy,  
66 and to develop suitable tools that will allow us to simulate and quantitatively evaluate the impacts of  
67 currently applied management practices, the potential impacts of future management practices, or the  
68 shifts in environmental conditions including changing land use and climate.

## 69 **1.2 Soil Organic matter and fertility**

70 Soil fertility strongly depends on soil organic matter (SOM) (Lal, 2015, 2004; Tiessen et al., 1994) by  
71 improving soil physical, chemical and biological properties that support primary production by  
72 vegetation. The formation of WSA favors the sequestration of C in the soils by protecting it from  
73 decomposition (Tisdall and Oades, 1982), reducing in this way CO<sub>2</sub> emissions to the atmosphere (Lal,  
74 2004). The distribution of aggregates between the different size classes has been related to soil  
75 structure, SOM and biological activity and represents soil's ability to resist disintegration by  
76 disruptive forces (Six et al., 2000). The formation of WSA due to OM addition, improves soil  
77 structure and the hydraulic properties of bulk soil through the formation of larger connected pores  
78 resulting in increased bulk permeability to fluid flow and improved drainage, while increasing the  
79 water holding capacity within the microscopic pores of the larger aggregates. WSA formation is  
80 directly related to protection of SOM. SOM can chemically bind to soil mineral particles, making  
81 SOM less bioavailable in sorbed form, and also altering the surface properties of soil mineral to

82 favour particle-particle binding and aggregation (Nikolaidis and Bidoglio, 2013). Formation of larger  
83 aggregates also provides a redox barrier by holding water within the microscopic pores of the  
84 aggregates, which creates a diffusion barrier to O<sub>2</sub> and protects the SOM against oxidative microbial  
85 degradation. On the other hand, soil structure is affected adversely by the mechanical shearing created  
86 by tillage, by freezing and thawing that results from extreme temperature fluctuations, and by the  
87 compaction that is due to the use of heavy machinery (Ross et al., 2015).

88 Restoration of soil fertility through soil management can be achieved by applying appropriate agro-  
89 ecological practices (Lal, 2013). Crop rotation, organic-C addition as SOM with associated nutrient  
90 elements, reduced tillage, use of cover crops during fallow periods, and controlled grazing are among  
91 the most commonly applied practices for sustainable agriculture (Milne et al., 2015). Incorporation of  
92 plant residues and organic amendments, such as compost and manure, combined with reduced tilling,  
93 enhance C sequestration (Lal, 2015) and plant production (Li et al., 2016; Liao et al., 2015) as well as  
94 soil hydraulic properties (hydraulic conductivity, water holding capacity, aeration, and porosity)  
95 (Udom et al., 2016). Field experiments with organic amendments have shown that manure improves  
96 soil structure and protection of aggregate-associated SOM much more than plant compost in terms of  
97 aggregate size and C content (Udom et al., 2016) while evidence has been provided that a mixture of  
98 compost (e.g. municipal solid waste derived) and manure (of a rate 70/30 respectively) is equally  
99 beneficial, resulting in the increase of the large (>250 µm) WSA mass fraction (Kotronakis et al.,  
100 2016; Udom et al., 2016). The effectiveness of these practices depends strongly on OM application  
101 rate and composition, climate, and other management practices.

### 102 **1.3 Modeling soil carbon and structure dynamics**

103 Mathematical models have been developed to simulate and predict soil structure development and C  
104 sequestration. These soil properties, as measured by WSA and soil C stocks and their rates of  
105 formation, provide proxy measures for soil fertility, defined here as the capacity of soil to support the  
106 rate of primary production by vegetation (e.g. g C fixed y<sup>-1</sup> kg soil<sup>-1</sup>). Over the past decades, several  
107 mathematical models were developed to simulate SOC dynamics. Mathematical models such as

108 CENTURY (Parton et al., 1987), Roth-C (Coleman, K., Jenkinson, 1999; Jenkinson, 1990), DNDC  
109 (Gilhespy et al., 2014; Li et al., 2005) and APSIM (Keating et al., 2003), have been used (Álvaro-  
110 Fuentes and Paustian, 2010; Andrianaki et al., 2016; Carvalho Leite et al., 2004; Dou et al., 2014;  
111 Galdos et al., 2009; GAO et al., 2008; Goglio et al., 2014; Luo et al., 2013; Poeplau and Don, 2015;  
112 Stamati et al., 2013b; Zhang et al., 2016) to assess the impact of land management on SOM stocks  
113 and to investigate the ability of these models to simulate long term (decades – centuries) SOM  
114 dynamics across different ecosystems (Smith et al., 1997). However, these models do not consider the  
115 effect of structure and its feedbacks on organic-C dynamics. Several studies have revealed a strong  
116 effect of structure on SOC turnover (Jastrow et al., 2007), identifying the link between OM  
117 decomposition and aggregate stability (Abiven et al., 2009), and summarizing the dynamics of SOC  
118 turnover with changes in soil structure (Nikolaidis and Bidoglio, 2013),. Existing models have been  
119 updated (Coleman and Jenkinson, 1999) or further modified (Jenkinson and Coleman, 2008; Nadeu et  
120 al., 2015), to incorporate the contribution of factors affecting SOC dynamics and aggregate formation.  
121 Over the last decade new models have been developed, and new conceptual frameworks on modeling  
122 of soil functions have been proposed. Abiven et al. (2008) developed the Pouloud model to predict the  
123 impact of organic residues incorporation on aggregate stability, under field conditions. The Struc-C  
124 model (Malamoud et al. 2009) was based on the RothC-26.3 model and linked SOM dynamics with  
125 soil aggregation and soil structure. The InVEST model (Nelson et al., 2009) was structured to predict  
126 changes in ecosystem services under different land use/land cover change scenarios, incorporating  
127 sub-routines assessing water service, soil conservation, C sequestration, biodiversity conservation and  
128 commodity production value. The SoilGen2 model (Finke, 2012), which is a further development of  
129 the SoilGen1 model (Finke and Hutson, 2008), is a 1D model that simulates the pedogenesis of  
130 various parent materials and includes clay formation, and has been used to successfully simulate soil  
131 formation. Segoli et al., (2013) developed the AggModel which is a combination of an aggregate  
132 dynamics model and a SOM dynamics model, where the C pools are not conceptual but directly  
133 measured. Finally, (Stamati et al., 2013a) developed the CAST model using an aggregation  
134 mechanism similar to the Struc-C model approach and modeling the carbon sequestration and  
135 turnover rates in each aggregate size.

136 The objective of this work is to use the results of the CAST model simulations of SOC and WSA  
137 dynamics for 7 sites around the world with different land use management practices, including natural  
138 and agricultural ecosystems, in order to characterize the process rates and the factors controlling soil  
139 structure dynamics and C sequestration across different climatic and lithological conditions. A meta-  
140 modeling Principal Component Analysis (PCA) integrates the results, clusters the sites by dominant  
141 factors influencing SOC and structure dynamics, and identifies the principal factors controlling C  
142 sequestration within the clustered sites.

## 143 **2. Methodology and methods**

144 The CAST model (Stamati et al., 2013a) was used to simulate soil structure dynamics and C  
145 sequestration in seven sites across the world. The sites were the Koiliaris CZO, Slavkov Forest CZO,  
146 Marchfeld CZO, Clear Creek (Iowa, USA), Damma Glacier CZO, Heilongjiang Mollisols (China) and  
147 Milia (Greece), representing various climates, land management practices, soil properties and  
148 histories. Table 1 presents the list of the natural ecosystems and agricultural fields of each study site.

149 [Insert Table 1 here]

150 The simulations of the CAST model from the Marchfeld CZO, Slavkov Forest CZO, and the  
151 agricultural fields of Koiliaris CZO and Clear Creek are presented, while the simulations of Damma  
152 Glacier CZO, Heilongjiang Mollisols, Milia and the natural ecosystems of Koiliaris CZO and Clear  
153 Creek are described previously (Andrianaki, 2016; Li et al., 2016; Stamati et al., 2013a; Vavlas et al.,  
154 2014). The geographic distribution of the sites evaluated in this work is shown in Figure 1.

155 [Insert Figure 1 here]

156 All model simulations were performed using consistent guidelines. The simulations were compared in  
157 terms of the stocks and flows of C taking into account C sequestration, microbial biomass and the  
158 CO<sub>2</sub> flux as well as the changes in the mass distribution of WSA size classes. A comparison of the  
159 sites was conducted regarding the rate constants related to the processes of plant biomass  
160 fragmentation, formation of micro- and macro-aggregates, SOC decomposition and aggregate

161 disruption. Finally, principal component analysis (PCA) was performed in order to identify the most  
162 significant model input, output and calibration parameters as the factors controlling SOC and soil  
163 structure dynamics and to identify sites across climatic and lithological gradients with similar  
164 responses to SOC sequestration. The model parameters that were included in the PCA analysis were  
165 selected based on a parameter sensitivity analysis conducted during the calibration process. The most  
166 sensitive (i.e. affecting the simulation results) input, output and model parameters were included in  
167 the PCA analysis. The PCA was performed using the MiniTab 17 statistical software.

## 168 **Methods**

### 169 **2.1 Model Description**

170 The CAST model simulates the mechanisms of aggregation assuming three size classes of aggregates:  
171 the silt-clay sized aggregates (AC1,  $< 53 \mu\text{m}$ ), the micro-aggregates (AC2;  $53\text{-}250 \mu\text{m}$ ) and the  
172 macro-aggregates (AC3,  $> 250 \mu\text{m}$ ). Figure 2 presents a schematic representation of the concept of  
173 WSA formation modified from Stamati et al. (2013). The model assumes that macro-aggregates are  
174 formed around large particulate organic matter (POM), followed by the inclusion of micro-aggregates  
175 within the macro-aggregates. Microbial decomposers of plant residues provide the extracellular  
176 polymeric “glue” by which mineral particles and small aggregates bind to form macro-aggregates  
177 around the POM (Phase I). Clay-sized mineral particles with relatively larger specific surface area  
178 provide complexation capacity to chemically bind constituent molecular components of SOM to the  
179 mineral surfaces, which protects the organic matter and favours inclusion of the clay-size fraction in  
180 micro- and macro-aggregate formation (Nikolaidis and Bidoglio, 2013). The macro-aggregate POM is  
181 further decomposed and the resulting finely fragmented POM is encrusted with silt-clay sized  
182 aggregates leading to the formation of micro-aggregates within macro-aggregates (AC2 in AC3)  
183 (Phase II). Decreased microbial activity inside the macro-aggregates due to decreased availability of  
184 C and energy following biodegradation of POM reduces the supply of microbial polymers and  
185 aggregate disruption occurs (Phase III) with instant release of stable AC2 and AC1 aggregates and the



186 fragmented POM becomes unprotected (Phase IV). When fresh plant residues enter the soil, new  
187 macro-aggregates form and the cycle of aggregation and dis-aggregation continues.

188 [Insert Figure 2 here]

189 Figure 3 presents a schematic representation of the aggregation process of the CAST model, its  
190 aggregate fractions and the C pools sequestered in them. Each arrow represents a mass transformation  
191 rate that is translated mathematically by the law of mass action into a linear rate equation with a first-  
192 order rate constant that defines the rate as proportional to the mass of the reactive material that is  
193 being transformed. The figure shows the phases of WSA formation together with the C pools and  
194 fluxes. Fresh plant residue is characterized by the decomposable (DPM) and resistant plant material  
195 (RPM). Both DPM and RPM are fragmented and comprise the coarse fraction of DPMc and RPMc  
196 which further break down to fine fractions DPMf and RPMf. In the initial phase of aggregation, the  
197 AC3 aggregates are comprised of POM, AC1 aggregates, sand, bacteria and fungi. At the second  
198 stage, coarse plant material, DPMc and RPMc is decomposed within the AC3 into fine, fragmented  
199 DPMf and RPMf which further facilitates the formation of the AC2 micro-aggregates within the AC3.  
200 Further biodegradation of the OM decreases the microbial activity and the stability of the macro-  
201 aggregates which eventually break down into aggregates of the AC1 and AC2 size fractions.

202 [Insert Figure 3 here]

203 The CAST model has been further modified to incorporate the effect of tilling and the impact of  
204 frozen soil on the aggregation/disaggregation mechanisms in order to improve the model versatility  
205 and extend the conditions that can be represented by simulation of the dynamics of SOM. Tilling was  
206 incorporated in the model by making the WSA destruction parameters time-variable. When there is  
207 tilling, the destruction rate parameter can be changed to a higher value, depending on the tilling  
208 intensity, which upon cessation of tilling subsequently reverts to its initial value. Similarly, frozen soil  
209 was incorporated into the model by allowing the rate constants of aggregation and decomposition of  
210 OM to vary with temperature. When the ground was defined as frozen, the rate constants of

211 aggregation and OM decomposition can be changed to lower values which, over time, can then revert  
212 to their normal values.

213 The most important input parameters of the CAST model include climatic data such as temperature,  
214 precipitation and evapotranspiration (ET), soil properties (silt and clay content and bulk density) and  
215 WSA distribution and SOC stock distribution within each of the defined fractions of WSA. More  
216 specifically, samples from the topsoil (0-10 cm) for each field site were analyzed for the AC1, AC2  
217 and AC3 fractions of WSA according to the methodology developed by Elliott (1986). AC3  
218 aggregates were further separated to coarse POM (POMc), sand, easily dispersed silt-clay fraction and  
219 AC2 aggregates according to Lichter et al. (2008). The AC2 aggregates within the AC3 aggregates  
220 were further separated into fine POM (POMf), sand and the silt-clay fractions. The free AC2  
221 aggregates were also separated into POMf and silt-clay fractions. These measurements are performed  
222 for every soil sample in order to obtain parameter values both for the initialization and calibration of  
223 the model.

## 224 **2.2 Site Description**

225 The data and experimental results used in the simulations represent conditions of natural ecosystems  
226 and agricultural practices. Table 2 presents a summary of the sites and their respective management.  
227 A description of the site details follows:

### 228 *Damma Glacier CZO – Switzerland*

229 Damma Glacier CZO is located at the central Alps, Canton Uri, Switzerland and is a 9.9 km<sup>2</sup>  
230 catchment with an elevation range between 1940 and 3630 m above sea level. The glacier has been  
231 retreating since 1850, forming a soil chronosequence on a relatively flat area of about 1 km length at  
232 an altitude between 1950 and 2050 m. The glacier recession was reversed two times, during 1920 to  
233 1928 and 1970 to 1992, which resulted in two small terminal moraines. Therefore, the  
234 chronosequence consists of three groups of soil ages. The youngest sites include soils from 6 to 14  
235 years old, the intermediate group comprises of soils developed between 1930 and 1950 and the oldest  
236 group includes soils that started to evolve during 1870 to 1897. The soils have been classified as

237 Lithic leptosols. The soils at locations in the chronosequence, between those representing these stages  
238 of soil formation, have been eroded during glacial advances (Banwart et al., 2011; Bernasconi et al.,  
239 2011). The CAST model was used to simulate the accumulation of SOC and the development of soil  
240 structure along the chronosequence (Andrianaki et al., 2016). As the chronosequence is not  
241 continuous there were 5 simulations, 3 of the different soil ages (young soils, intermediate soils and  
242 old soils) and 2 of the readmissions of the glacier. The calibration of the models is based on the  
243 extensive dataset available for the Damma Glacier CZO and a climate reconstruction back to 1867  
244 (Smittenberg et al., 2012).

#### 245 *Heilongjiang Mollisols – China*

246 The Heilongjiang Mollisols experimental field site is located in the central region of the Mollisols in  
247 Northeast China. The experimental site was established in 2004 at the State Key Experimental Station  
248 of Agroecology, Chinese Academy of Sciences, Hailun, Heilongjiang province. The region has a  
249 typical temperate continental monsoon climate with a hot summer and cold winter. The soils have  
250 evolved from sedimentary materials of loamy loess. Parent material was removed from the C horizon  
251 (> 2 m) and replaced the surface soil down to 0.8 m. The experiment was set up to study soil  
252 development and restoration from an extremely degraded soil (Li et al., 2016). The field experiment  
253 included six treatments, two natural ecosystems and four agricultural fields, in order to compare: a)  
254 no-tilled soils under fallow and soil planted with alfalfa and b) tilled soils with rotation of soya and  
255 maize in alternate years and different combinations of mineral fertilization (F) and organic (C)  
256 amendments. More specifically the tilled soils were managed i) without fertilization and organic  
257 amendment (F0C0) after the above-ground biomass was removed, ii) with fertilization and no organic  
258 C amendment (F1C0), iii) with fertilization and low amount of organic C input (F1C1) after only  
259 partial above-ground biomass of two crops was incorporated into soil, and iv) with fertilization and  
260 high amount of organic C input (F1C2) after all the above-ground biomass of the seasonal crop was  
261 incorporated into the soil (Li et al., 2016).

262 *Koiliaris CZO – Greece*

263 Koiliaris River catchment is a CZO that represents severely degraded soils due to intense agricultural  
264 practices applied for many centuries. It represents typical Mediterranean dry-lands soils evolving  
265 under imminent threat of desertification. The Koiliaris CZO is located 25 km east of the city of  
266 Chania, Crete, Greece. The total watershed area is approximately 130 km<sup>2</sup> and the main supply of  
267 water originates from the White Mountains. An additional area of 50 km<sup>2</sup> outside of the Koiliaris  
268 CZO is hydro-geologically connected due to limestone bedrock-karst terrain. Water erosion is  
269 recognized as the most important soil degrading threat due to the clearing of forests and natural  
270 vegetation, the livestock overgrazing and the tilling of crops (Stamati et al., 2013a, 2013b).  
271 Simulations performed for the Koiliaris CZO included both natural ecosystem and agricultural  
272 management scenarios and the soil type is calcaric regosol.

273 *Clear Creek – Iowa, USA*

274 The Clear Creek site is located on the outskirts of Iowa City, USA. It is representative of humid  
275 continental climates with coarse textured (sandy loam) Mollisols. The cropping period lasts from May  
276 to September, while during the winter period the soils are covered by snow. The site has been selected  
277 to study the impacts of land use conversion, from agricultural use to natural vegetation, on soil  
278 functions (Stamati et al., 2013a, 2013b).

279 *Slavkov Forest CZO – Czech Republic*

280 Slavkov Forest CZO is a Protected Landscape Area located in the northwestern Czech Republic, 120  
281 km west of Prague. The catchment area is 0.273 km<sup>2</sup>, with elevations in the range of 829 to 949 m  
282 above sea level. There is intense silviculture with rapidly aggrading Norway spruce monoculture  
283 stands since 1850 on nutrient-depleted soils, mostly Podzols developed on granite. The mean stand  
284 age is about 40 years, and closed canopy forest covers 82% of the CZO, while clearings with young  
285 seedlings cover 18% of the catchment. The most important threats to the soil include nutrient  
286 leaching, acidity, metal toxicity, harvest erosion and compaction, low biodiversity due to  
287 monoculture, C loss due to elevated organic C export and atmospheric deposition of anthropogenic  
288 pollutants (Banwart et al., 2011).

289 *Marchfeld CZO – Austria*

290 The study area is located in the Danube River flood plain downstream of Vienna in the “Marchfeld”,  
291 with little variation in topography and climate. During alpine glaciations, the Danube continuously  
292 incised into the uplifting Tertiary basin fill and accumulated melt water terraces. The floodplain is  
293 morphologically subdivided into two units: the recent floodplain sensu stricto and a slightly elevated  
294 area covered by older fluvial deposits. The soils in the Marchfeld CZO are Chernozems and create a  
295 chronosequence of soil development covering thousands of years, which allows the study of temporal  
296 soil development and also the effects of various land uses. The data from Marchfeld CZO were used  
297 to perform three simulations of the land use conversion (Rampazzo Todorovic et al., 2014). The initial  
298 conditions for each case are freshly deposited sediments with specified soil texture but without  
299 structure. Every simulation represents the evolution of C sequestration and soil structure development.  
300 The first 200 years of each simulation represent the forest development. The term “*Forest*” refers to  
301 the simulation of subsequent steady-state climax forest for 400 years. The term “*Cropland*” refers to  
302 the simulation of land use conversion from forest (initial 200 years) to cropland (total 400 years), and  
303 the term “*Grassland*” refers to the simulation of land use conversion from forest (initial 200 years) to  
304 grassland (total 400 years). The lengths of these periods were inferred from land use history.

305 *Milia – Greece*

306 Milia represents a strongly eroded Eutric Lithosol soil in which restoration practices including  
307 terraces formation and incorporation of organic amendments have been applied. The elevation of the  
308 study area is 500 m above sea level. Soil samples were collected from three terraces subjected to  
309 cultivation with varying compost application practices. Simulations were performed to represent a 10  
310 year period of farming operations (Vavlas et al., 2014). The frequency of compost application was  
311 twice per year, through tilling, corresponding to a total application of 8 t C/ha. For terrace 1 (Milia 1),  
312 the compost was applied annually for 10 years, while for terrace 2 (Milia 2) it was applied for 8 years  
313 followed by 2-years fallow. Finally, for terrace 3 (Milia 3), the organic amendment was applied once  
314 every 3 years.

315 [Insert Table 2 here]

### 316 **3. Results and Discussion**

317 The interpretation of soil properties, climatic conditions, and land use and management practices in  
318 the study areas reveals great variability. The sites are characterized by variable climatic conditions  
319 ranging from 0-4 °C of mean annual temperature of Damma Glacier CZO to 17.6-18.1 °C of the  
320 Greek sites. Precipitation also varies from 1898 mm/yr of Damma Glacier CZO to 510 mm/yr of the  
321 Heilongjiang Mollisols. In addition, the sites cover a wide variety of soil types at different stages of  
322 soil development, from lithic leptosol of Damma Glacier to eutric lithosols of Milia, to calcareous  
323 regosols of Koiliaris and then to more developed podsoles, chernozems and mollisols of Slavkov  
324 forest, Marchfeld and China/USA respectively. Organic carbon input to the soils at the natural  
325 ecosystem sites was approximately proportional to the temperature gradient as it is shown in the site  
326 data comparison of Table 3. The lowest C inputs occurred at the Damma Glacier CZO and the  
327 Heilongjiang Mollisols and approached 1 t C/ha/yr as a consequence of the short growing season  
328 imposed by the low temperatures. As the annual average temperature increases to 5.3 °C in Slavkov  
329 Forest CZO, the C input also increased to 2.75 t C/ha/yr. For higher temperatures, such as that of  
330 Clear Creek with 10.3 °C and of Koiliaris CZO 18.1 °C, the amount of C inputs was strongly mediated  
331 by the precipitation level and its seasonal distribution. For instance, the C input of Clear Creek was  
332 5.8 t C/ha/yr due to the availability of precipitation during the summer (923 mm/yr) whereas in  
333 Koiliaris CZO is 3.8 t C/ha/yr due to semi-arid climate (652 mm/yr). Organic carbon input to soils at  
334 the agricultural sites depends on the applied management practices; e.g. tilling intensity, below  
335 ground biomass of from crop production, and the amount of above ground biomass incorporated to  
336 the soil. At these sites, annual C input varies from 0.205 tC/ha at Marchfeld to 8 tC/ha at Milia.

337 [Insert Table 3 here horizontally]

338 A schematic diagram of the study sites placed along a temperature gradient representing different  
339 stages of soil evolution is illustrated in Figure 4. The sites are placed according to the annual mean  
340 temperature, beginning from the Heilongjiang Mollisols and Damma Glacier CZO, to Slavkov Forest  
341 CZO, Marchfeld CZO, Clear Creek ending to Milia and Koiliaris CZO. The initial soil conditions for  
342 the model simulations of each site, in terms of clay and macro-aggregate content, and the rates of

343 macro-aggregates formation and decomposition of plant litter are also illustrated in Figure 4. The  
344 insert in each site are the C flux balances which include C input, C storage and CO<sub>2</sub> emissions. The  
345 ordering of sites according to temperature also coincides with the different stages of soil evolution  
346 starting from soil formation due to weathering in Damma Glacier CZO and the parent material of  
347 Heilongjiang Mollisols, moving to soils used for forestry at Slavkov Forest CZO and arable land at  
348 Marchfeld CZO, ending at the relatively degraded soils of Clear Creek and Koiliaris CZO due to  
349 permanent cropping and overgrazing. The C flux balances show soil degradation due to C losses  
350 represented by the negative values of C storage. The site of Milia is placed outside the circle of soil  
351 formation and soil degradation because it represents soil restoration conditions due to organic carbon  
352 addition.

353 [Insert Figure 4 here]

### 354 **3.1 Calibration results**

355 The simulations for the Koiliaris CZO, Clear Creek, Marchfeld CZO, and Slavkov Forest CZO sites  
356 with regard to the distribution of SOC stocks and WAS, and their interpretation with the field data  
357 used for model calibration, are shown in Figure 5a and Figure 5b respectively. The calibration  
358 parameters of the CAST model and their description are summarized in Table 4. The descriptions of  
359 the parameters indicating soil initial conditions are presented in Table SI 1 (Appendix –  
360 Supplementary Information).

361 [Insert Table 4 here]

362 [Insert Figure 5a here]

363 [Insert Figure 5b here]

364 A comparison of the CO<sub>2</sub> fluxes, C stocks, and microbial biomass is presented in Table 5. The table  
365 presents the initial C content of each site that ranges from 0.6-14.8 t C/ha at Damma Glacier CZO to  
366 13.5 t C/ha for the Heilongjiang Mollisols to 55.4 t C/ha for Slavkov Forest, to 18.5 t C/ha for Clear  
367 Creek and 34.9 t C/ha for Koiliaris CZO soil, for the natural sites. Regarding the agricultural sites, the  
368 initial SOC mass ranges from 13.77 t C/ha for the Heilongjiang Mollisols to 58.55 t C/ha for Koiliaris

369 CZO soil. Milia had an initial SOC mass of 33.9 t C/ha, Clear Creek 32.38 t C/ha and Marchfeld CZO  
370 27.11 t C/ha. The values of initial SOC mass of Damma Glacier CZO and Heilongjiang Mollisols can  
371 be explained by the fact that Damma Glacier CZO is a very new, 150-year-old, soil, while the  
372 Heilongjiang Mollisols were C horizon soil brought to the soil surface and placed under cultivation.  
373 The high value for Slavkov Forest CZO is due to the fact that it is a forested site relatively  
374 undisturbed for the past 70 years, while the low value of Clear Creek is due to intense cultivation of  
375 the Iowa, USA soils and the sandy / low clay content nature of the soil that offers limited mineral  
376 surface for binding and forming organo-mineral complexes that protect and sequester OM. Finally,  
377 the initial SOC mass of Koiliaris CZO is indicative of its relatively high clay content and lower  
378 intensity of agricultural practices.

379 [Insert Table 5 here horizontally]

380 Regarding the natural ecosystems, the young soils of Damma Glacier CZO and Heilongjiang  
381 Mollisols sequester higher amounts of the C input, up to 0.31 (28%) and 0.47 t C/h/yr (40%)  
382 respectively, while the older soils of the Clear Creek and Koiliaris CZO sequester significant lower  
383 proportions, 5% and 13% respectively even though the annual storage is maintained close to that of  
384 the young soils (0.27 t C/ha/yr for Clear Creek and 0.48 t C/ha/yr for Koiliaris CZO). These  
385 differences can be explained by climatic conditions, soil structure and land use management. Slavkov  
386 Forest CZO presents intermediate values with 26% (0.72 t C/ha/yr) of the C input to sequestered  
387 annually. The CO<sub>2</sub> emissions follow the opposite trend to that observed for C storage with the young  
388 soils having lower emissions compared to the older soils. As for the cultivated sites, the initial SOC  
389 mass (Table 3) ranged from 13.77 t C/ha for the Heilongjiang Mollisols to 58.55 t C/ha for Koiliaris  
390 CZO soil. Milia had an initial SOC mass of 33.9 t C/ha, Clear Creek 32.38 t C/ha and Marchfeld CZO  
391 27.11 t C/ha. The values of initial SOC mass of Heilongjiang Mollisols can be explained by the fact  
392 that the Heilongjiang Mollisols had a well-developed C horizon when the cultivation started. C input  
393 ranged from 0.2 t C/ha at Marchfeld to 8 t C/ha in Milia. The data from the Heilongjiang Mollisols  
394 showed that the higher the C input, the more the C storage, CO<sub>2</sub> emissions and bacterial biomass. A  
395 similar trend was found for the Milia soils. Comparison of sites with similar C input such as the



396 Koiliaris CZO and Marchfeld CZO revealed that climate (i.e. temperature, rainfall) and water  
397 availability through irrigation played an important role. The warmer site (Koiliaris CZO) showed  
398 higher CO<sub>2</sub> emissions and loss of organic C despite the lower bacterial stock. Similar emissions of  
399 CO<sub>2</sub> to those observed in the Koiliaris CZO were observed in the Heilongjiang Mollisols which could  
400 be attributed to the higher C input.

401 The poor soil structure of the Heilongjiang Mollisols and the Damma Glacier CZO seems to improve  
402 with time. This is evident in the Damma Glacier CZO chronosequence where the macro-aggregate  
403 AC3 fraction increases from 15% to 46%. In the Heilongjiang Mollisols the macro-aggregate fraction  
404 ranged between 29-35%. Even greater proportions of macro-aggregates were found in the Clear Creek  
405 and Slavkov Forest CZO soils that approached 79% and 78% respectively. The corresponding  
406 proportion for the Koiliaris CZO scrublands was 47%. Finally, in the forests and grasslands of the  
407 Marchfeld CZO the macro-aggregate fraction was 45% and 57% respectively.

408 Regarding the cultivated sites, the Heilongjiang Mollisols macro-aggregate fraction ranged from 21%  
409 to 48% depending on the management practice. Milia macro-aggregate fractions ranged from 45% to  
410 70% with the highest proportions corresponding to the treatment of the annual application of organic  
411 matter amendment. Finally, the Koiliaris CZO macro-aggregate fraction was 53%, Clear Creek was  
412 74% and Marchfeld CZO was 23%, again reflecting differences regarding climate, agricultural  
413 practices and soil properties. A decrease in the macro-aggregate fractionation was observed in  
414 Koiliaris CZO natural ecosystem, which was accompanied by an increase in the micro-aggregate  
415 fraction AC2. The site of Marchfeld CZO showed a large (277%) increase in AC3 content the first  
416 200 years of forest development, since the site initially was consisted of sediment depositions, with no  
417 aggregates and soil structure.

418 The values for the calibration parameters of the CAST model for the simulations of natural  
419 ecosystems and agricultural sites are summarized in Table SI 2 and Table SI 3 respectively, while a  
420 range of these values is presented in Table SI 4 in order to provide an initial database for future  
421 modeling activities. Overall, the modeling results of the CAST model for both the natural ecosystems

422 and agricultural management sites were consistent with the field data. The model has been able to  
423 describe SOC and soil structure dynamics in a wide variety of natural ecosystem and agricultural sites  
424 around the world. A broad comparison between the process rates constants of the agricultural  
425 management sites and the natural ecosystems shows that the rates of fragmentation, micro aggregation  
426 and disruption are higher for the agricultural sites, while the rates for macro aggregation and  
427 decomposition of organic matter are higher for the natural ecosystems.

### 428 **3.2 Factors controlling soil structure dynamics and carbon sequestration**

429 Our findings confirmed those of earlier studies that the factors regulating the sequestration of C in  
430 soils are driven by complex interactions within the soil-plant-water system. A principal component  
431 statistical analysis (PCA) was employed to classify the soils studied in the present work in terms of  
432 their status considering climatic parameters, basic soil properties, SOC and macro-aggregate content  
433 at the initial and final stages of simulation and their annual rates of change, C input rates to soil  
434 through litter fall and organic amendments, the decomposition rates of the soil C pools, and the  
435 magnitude of disruption of the aggregates including the impact of tilling.

436 The score and the loading plots of the components of the PCA are presented in Figures 6 and 7 in  
437 order to illustrate the clustering of the sites and the significance of each parameter in this clustering.  
438 The 35 parameters used in the PCA together with the eigenvalues for the first two principal  
439 components are summarized in Table SI 5. The most important parameters that explained the  
440 variability in the first component are: the initial macro-aggregate fraction as percentage of total mass,  
441 the initial value of the SOC normalized to the mass content of the silt and clay, the temperature, the  
442 bulk density and the ET. Similarly, the most important parameters included in the second component  
443 are: the percent mass fraction of macro-aggregates, the percent mass fraction of silt-sized aggregates,  
444 the decomposition rates of humified and bacterial organic C pools, and the fragmentation rate of  
445 resistant plant material by soil fauna. PC1 could explain 32.1% of the variability of the samples, while  
446 together with PC2 49.7% of the variability.

447 Figure 6 presents the clustering of the sites as a result of the PCA. A plot of PC1 versus PC2 of all the  
448 sites resulted in the development of four clusters. The first cluster includes the sites of Heilongjiang  
449 Mollisols (all management practices) and Damma Glacier CZO (new and intermediate soils) which  
450 represents soils at their early stage of evolution. For the Heilongjiang Mollisols, this reflects the  
451 introduction of C horizon parent material to the soil surface, hence exhibiting characteristics of a  
452 young soil. The second cluster includes all the sites of Marchfeld CZO, Slavkov Forest CZO, Damma  
453 Glacier CZO (older soils) and the natural ecosystems of Koiliaris CZO. These sites are either natural  
454 or set aside sites or flood plain soils with a high degree of fertility. The third cluster includes the  
455 agricultural sites of the Koiliaris CZO and all the Clear Creek studies which represent intensively  
456 managed soils. Finally, the fourth cluster includes the site of Milia (all management practices) where  
457 intensive C sequestration occurs due to large C additions. As it can be seen from Figure 6, PC1  
458 differentiates the sites starting from the left with soils at an early stage of evolution, moving to the  
459 second cluster in the middle with mature soils and moving to the upper right of the graph with the  
460 intensively managed soils. PC2 differentiates the sites based on the degree of intensification versus  
461 natural ecosystem sites but with C addition. Cluster 4 accounts for the Milia site which diverges from  
462 the main trend of clusters 1 through 3 due to extensive C addition. Similarly, the sites within cluster  
463 1 identify a trend from the early diagenesis sites of Damma Glacier CZO to the cultivated C horizon  
464 sites of the Heilongjiang Mollisols. It is interesting to note that PC2 differentiates the Chinese  
465 Heilongjiang Mollisols based on the amount of C added.

466 [Insert Figure 6 here]

467 In terms of soil carbon evolution, the four clusters of Figure 6 represent the sites dominated by carbon  
468 fixation (Cluster 1), the sites with stable SOC content (Cluster 2), the sites dominated by SOC  
469 mineralization and net loss (Cluster 3) and the sites with large artificial SOC addition (Cluster 4).

470 Figure 7 presents the Loading Plot of the PCA analysis in order to identify the most important  
471 parameters contributing to the differentiation of the clusters. The factors contributing to the  
472 differentiation of Cluster 1 includes bacterial biomass as a proxy for microbial decomposer activity,

473 SOC storage, the increase of the fertility factor  $SOC/(silt + clay)$  and the increase of the macro-  
474 aggregate fraction. Cluster 2 represents older soils which have probably reached a steady state. This  
475 cluster is placed in the middle of the diagram where all the factors play a seemingly equal role.  
476 Cluster 3 represents degraded soils where the decomposition rates of the C pools is higher, the  
477 decomposable plant material outweighs the resistant plant material and the disruption of macro-  
478 aggregates is increased. Cluster 4 represents soils restored by beneficial intervention practices where  
479 the aggregation rates are higher, the plant material is decomposed by fauna and contributes to  
480 aggregation. The trend presented in the PCA analysis in Figure 6 is related to the evolutionary nature  
481 of the soils beginning from the young soils and parent material, proceeding to the older soils, forests  
482 and arable lands, ending either at soil degradation through continuous cultivation or to restoration  
483 through beneficial practices of previously intensively managed soils. In broad terms the evolution of  
484 soil structure and increasing intensity of human exploitation of the resulting soil functions correlates  
485 with the trajectory shown in Figure 6. This trajectory starts from young soils at the left, to productive  
486 soils in the centre, to heavily impacted and very intensively managed soils at the upper right. The  
487 dotted arrows show the trend of soil evolution within each CZO. For the Heilongjiang Mollisols, the  
488 trend starts at the natural ecosystems ending at the cultivation practices. For the Damma Glacier CZO  
489 soils, it begins at the young soils, ending at the older soils. For the Marchfeld CZO soils the trend  
490 starts at the grassland, moving to forest, ending at the agricultural land. At Koiliaris CZO and Clear  
491 Creek the trend starts at natural ecosystem ending at cultivation. At Milia the trend of soil restoration  
492 starts at low C amendment addition ending at higher application. It appears that the first two principal  
493 components can account for the variability that describes the evolutionary nature of soil from  
494 formation to cultivation as well as a reverse in this trajectory when moving from intensive utilization  
495 with soil degradation to restoration.

496 [Insert Figure 7 here]

497 Figure 7 presents the variables with the higher values, either positive or negative, of the factors with  
498 the higher impact on soil structure dynamics and C sequestration. These variables include soil bulk  
499 density, clay content, temperature, ET, initial SOC mass and AC3 fraction, decomposition rates of the

500 BIO and HUM pools, the contribution of plant litter and silt clay sized aggregates on AC2 and AC3  
501 formation, the formation rate of AC3 aggregates and the fragmentation of resistant plant material  
502 through fauna. Briefly the factors controlling soil structure and C dynamics are related to soil  
503 properties, climatic conditions, decomposition rates of organic matter, and formation rates and the  
504 predominant buildersers of macro aggregates.

#### 505 **4. Conclusions**

506 In this study, the CAST model was modified to incorporate the impact of tilling and frozen soil  
507 conditions on aggregate formation and SOC sequestration. The modified CAST model was used to  
508 simulate 20 cases of different soil management practices located at 7 sites across a wide range of  
509 climatic conditions, land uses, and parent material. The CAST model can successfully simulate and  
510 predict aggregate formation and C sequestration on soils across the world, under a variety of climatic,  
511 lithological and agricultural conditions. The principal component analysis indicated the predominant  
512 factors controlling soils structure and C sequestration to be the plant litter contribution to aggregate  
513 formation, the decomposition rates of the humified and bacterial C pools, the initial state of soil in  
514 terms of SOC, silt and clay and macro-aggregate contents, the fragmentation rate of plant material  
515 through earthworms and other fauna, the macro-aggregate formation rates, the temperature and  
516 evapotranspiration and the soil bulk density. The model reliably simulated soil C and soil structure  
517 dynamics for a wide variety of land uses, climatic and lithological conditions and soil properties  
518 providing support for the underlying conceptual and mathematical model and evidence that the CAST  
519 model provides a valuable quantitative analysis tool to interpret soil structure formation processes and  
520 to aid the design of sustainable soil management practices which support WSA formation.

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524

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<b>1. Table 1: Natural ecosystems (non tilled soils) and agricultural fields (tilled soils) of the study sites</b>	
<b>2. Natural Ecosystems</b>	<b>3. Agricultural Fields</b>
4. Koiliaris CZO – Calcaric Regosols - Set aside field	5. Koiliaris CZO – Calcaric Regosols - Cropland
6. Marchfeld CZO – Chernozems - Forest development	8. Marchfeld CZO – Chernozems -Land use conversion from forest to cropland
7. Marchfeld CZO – Chernozems - Land use conversion from forest to grassland	
9. Slavkov Forest CZO – Podsoles - Forestry	10.
11. Damma Glacier CZO - Lithic Leptosols	12.
13. Heilongjiang Mollisols: 2 fields with Natural Fallow and Alfalfa	14. Heilongjiang Mollisols: 4 fields with Soybean –Maize rotation
15. Clear Creek – Millisols - Set aside field	16. Clear Creek – Mollisols - Cropland
17.	18. Milia: Eutric Lithosols - 3 fields with different practices of compost application - Tilling

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**Table 2: Summary of sites simulated with a description of soil management**

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Site - Treatment	Description
Heilongjiang Mollisols - NatF	Natural fallow – No fertilization, Organic Input, No Tilling
Heilongjiang Mollisols - Alfa	Alfalfa – No fertilization, Organic Input, No Tilling
Heilongjiang Mollisols - F0C0	Soybean-maize rotation — No fertilization, No Organic Input, Tilling
Heilongjiang Mollisols - F1C0	Soybean-maize rotation — Fertilization, No Organic Input, Tilling
Heilongjiang Mollisols - F1C1	Soybean-maize rotation — Fertilization, Low Organic Input, Tilling
Heilongjiang Mollisols - F1C2	Soybean-maize rotation — Fertilization, High Organic Input, Tilling
Koiliaris Natural	Koiliaris set aside
Koiliaris Agricultural	Koiliaris agricultural management – Green vegetable, Light Tilling
Clear Creek Natural	Clear Creek set aside
Clear Creek Agricultural	Clear Creek agricultural management – Corn and Soybeans, Tilling
Milia1	Milia terrace 1 - compost application for 10 years, every year
Milia2	Milia terrace 2 - compost application for 8 years, every year and then fallow for 2 years
Milia3	Milia terrace 3 - compost application for 10 years, every 3 <sup>d</sup> year
Damma Young	Young soils of Damma Glacier CZO - ages from 6 to 14 years old
Damma Intermediate	Intermediate soils of Damma Glacier CZO - ages from 57 to 79 years old
Damma Old	Old soils of Damma Glacier CZO - ages from 108 to 140 years old
Marchfeld Forest	Marchfeld forest development (0 - 400 years forest)
Marchfeld Grassland	Marchfeld land use conversion from forest to grassland (0 - 200 year forest – 200-400 year grassland)
Marchfeld Agricultural	Marchfeld land use conversion from forest to cropland (0 - 200 year forest – 200-400 year cropland)
Slavkov Forest	Slavkov Forest CZO - Forestry

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**Table 3: Comparison of the site data: SOC, Soil Characteristics and Meteorological data**

<i>Site</i>	<i>Soil characteristics</i>			<i>SOC characteristics</i>		<i>Meteorological Data</i>		
	<i>Bulk Density</i> <i>(gr/cm<sup>3</sup>)</i>	<i>Silt clay</i> <i>(%)</i>	<i>Clay</i> <i>(%)</i>	<i>DPM to</i> <i>RPM ratio</i>	<i>Initial SOC</i> <i>mass</i> <i>(t C/ha-yr)</i>	<i>Mean</i> <i>Temperature</i> <i>(°C)</i>	<i>Mean</i> <i>Precipitation</i> <i>(mm)</i>	<i>Mean Pan</i> <i>Evaporation</i> <i>(mm)</i>
Heilongjiang Mollisols Alfa	1.35	77.6	42.0	0.25	13.77	2.5	510.6	514
Heilongjiang Mollisols NatF	“	“	“	0.15	“	“	“	“
Heilongjiang Mollisols F0C0	“	“	“	0.40	“	“	“	“
Heilongjiang Mollisols F1C0	“	“	“	1.00	“	“	“	“
Heilongjiang Mollisols F1C1	“	“	“	1.20	“	“	“	“
Heilongjiang Mollisols F1C2	“	“	“	1.44	“	“	“	“
Koiliaris CZO Natural	1.18	67.0	30.0	0.67	34.92	18.1	651.9	1916
Koiliaris CZO Agricultural	1.11	“	“	1.44	58.55	“	“	“
Milia 1	1.00	34.0	3.30	0.43	33.90	17.6	1494.6	1601.7
Milia 2	“	“	“	“	“	“	“	“
Milia 3	“	“	“	“	“	“	“	“
Clear Creek Natural	1.11	37.0	7.00	1.51	18.52	10.3	923.0	1413.6
Clear Creek Agricultural	“	“	“	2.00	32.38	“	“	“
Slavkov Forest CZO	1.30	47.0	11.00	0.25	55.36	5.3	1049.0	442.7
Marchfeld CZO Forest	2.00	73.6	16.36	0.25	20.00	9.1	687,0	727,7



Marchfeld CZO Grassland	1.26	“	“	0.70	27.11	“	“	“
Marchfeld CZO Cropland	1.26	“	“	1.44	“	“	“	“
Damma Glacier CZO Young Soils	1.50	35.0	3.10	1.44	0.60	4.0	1898.3	242.7
Damma Glacier CZO Intermediate Soils	1.50	“	“	“	1.05	2.9	“	“
Damma Glacier CZO Old soils	1.00	“	“	“	13.5	2.7	“	“

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DPM = decomposable plant material

RPM = resistant plant material

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**Table 4: Description of the Calibration Parameters of the CAST model**

<b>Main CAST model calibration parameters</b>		<b>Description</b>
<i>Fragmentation</i>	RPM to RPMc	Rate constant of fragmentation of Resistant Plant Material to coarse Resistant Plant Material
	RPMc to RPMf	Rate constant of fragmentation of coarse Resistant Plant Material to fine Resistant Plant Material
	RPMc(AC3) to RPMf(AC3)	Rate constant of fragmentation of coarse Resistant Plant Material to fine Resistant Plant Material within macro-aggregates
	DPMc(AC3) to DPMf(AC3)	Rate constant of fragmentation of coarse Decomposable Plant Material to fine Decomposable Plant Material within macro-aggregates
<i>Macroaggregation</i>	RPMc	Rate constant of coarse resistant plant material mass transfer for macro aggregate formation
	DPMc	Rate constant of coarse decomposable plant material mass transfer for macro aggregate formation
<i>Microaggregation</i>	RPMf(AC2inAC3)	Rate constant of fine resistant plant material mass transfer for micro aggregate formation within the macro aggregates
	DPMf(AC2inAC3)	Rate constant of fine decomposable plant material mass transfer for micro aggregate formation within the macro aggregates
<i>Decomposition</i>	fresh plant input(DPM)	Rate constant of decomposition of decomposable plant material from the plant litter pool
	BIO(AC1) within AC3	Rate constant of decomposition of Biomass carbon pools in Aggregate type 1 within Aggregate Type 3 (AC1 <sub>withinAC3</sub> )
	HUM(AC1) within AC3	Rate constant of decomposition of Humus in Aggregate type 1 within Aggregate Type 3 (AC1 <sub>withinAC3</sub> )
	BIO(AC2) within AC3	Rate constant of decomposition of Biomass carbon pools in Aggregate type 2 within Aggregate Type 3 (AC2 <sub>withinAC3</sub> )
	HUM(AC2) within AC3	Rate constant of decomposition of Humus in Aggregate type 2 within Aggregate Type 3 (AC2 <sub>withinAC3</sub> )

	BIO(AC2)	Rate constant of decomposition of Biomass carbon pools in Aggregate type 2
	HUM(AC2)	Rate constant of decomposition of Humus in Aggregate type 2
	BIO(AC1)	Rate constant of decomposition of Biomass carbon pools in Aggregate type 1
	HUM(AC1)	Rate constant of decomposition of Humus in Aggregate type 1
<i>Contribution in macroaggregation</i>	RPM <sub>c</sub>	Percent composition of macro aggregates (AC3) by coarse resistant plant material
	DPM <sub>c</sub>	Percent composition of macro aggregates (AC3) by coarse decomposable plant material
	AC1	Percent composition of macro aggregates (AC3) by silt clay sized aggregates (AC1)
	AC2	Percent composition of macro aggregates (AC3) by micro aggregates (AC2)
<i>Contribution in microaggregation</i>	RPM <sub>f</sub> within AC3	Percent composition of micro aggregates (AC2) by fine resistant plant material within macro aggregates (AC3)
	DPM <sub>f</sub> withinAC3	Percent composition of micro aggregates (AC2) by fine decomposable plant material within macro aggregates (AC3)
	AC1within AC3	Percent composition of micro aggregates (AC2) by silt clay sized aggregates (AC1) within macro aggregates (AC3)
<i>Disruption</i>	DPM <sub>f</sub> +DPM <sub>c</sub> within AC3	fine and coarse DPM pool contents of the AC3 aggregate type, below which macro-aggregates are considered unstable
	DPM <sub>f</sub> +DPM <sub>c</sub> AC2 within AC3	fine and coarse DPM pool contents of the AC2 aggregate type within AC3 aggregate type, below which micro aggregates within macro aggregates are considered unstable
	DPM <sub>f</sub> +DPM <sub>c</sub> within AC2	fine and coarse DPM pool contents of the AC2 aggregate type, below which micro-aggregates are considered unstable

**Table 5: Comparison of simulation results with regard to: Annual C stock and fluxes**

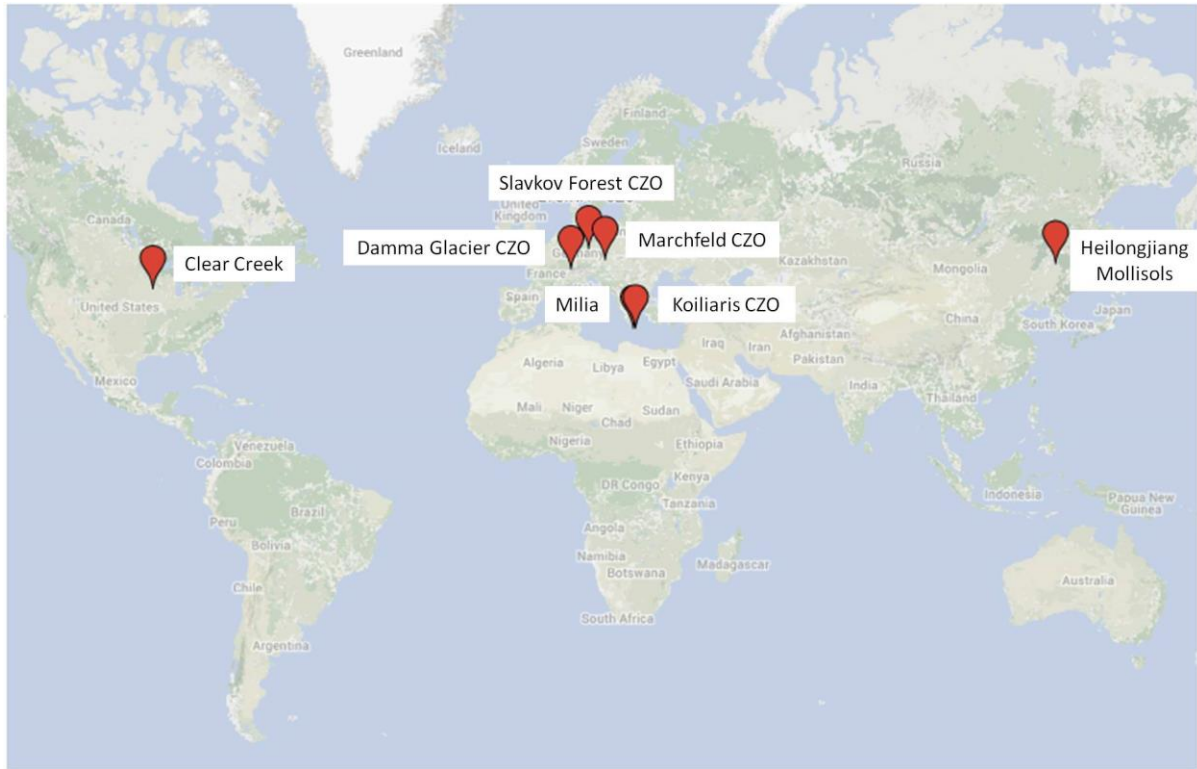
Site	Simulation period (y)	Annual C Input (t C/ha/yr)			Annual C Storage (t C/ha/yr)			Annual CO <sub>2</sub> emissions (t C/ha/yr)			Bacterial Stock (BIO - t C/ha/yr)	
		Average	min	max	Average	min	max	Average	min	max	Average	% of total stock
Heilongjiang Mollisols - NatF	10	0.76	0.00	0.95	0.37	-0.61	1.12	0.33	0.08	0.49	8.00	4.49
Heilongjiang Mollisols - Alfa	“	0.94	“	1.17	0.47	“	1.31	0.41	0.11	0.57	8.35	4.52
Heilongjiang Mollisols - F0C0	“	0.69	“	0.86	0.26	-0.54	0.65	0.38	0.11	0.6	8.51	4.92
Heilongjiang Mollisols - F1C0	“	1.05	“	1.31	0.32	“	0.71	0.67	0.26	1.15	10.17	5.72
Heilongjiang Mollisols - F1C1	“	2.27	“	2.84	0.84	“	1.57	1.36	0.26	2.43	13.6	6.51
Heilongjiang Mollisols - F1C2	“	2.96	“	3.70	0.99	“	2.42	1.89	0.26	3.69	16.18	7.30
Koiliaris CZO Natural	100	3.80	3.80	3.80	0.48	-0.8	1.07	3.29	2.73	4.47	15.8	2.10
Koiliaris CZO Agricultural	40	0.36	0.36	0.36	-0.65	-2.34	-0.31	0.92	0.57	2.58	11.60	2.30
Milia 1	20	8.00	8.00	8.00	2.16	0.28	4.29	5.64	2.61	7.72	39.80	5.54
Milia 2	“	3.20	0.00	“	-0.21	-5.59	4.29	3.2	1.23	5.59	30.76	5.98
Milia 3	“	1.20	0.00	“	-0.65	-5.58	5.72	1.65	0.66	3.09	18.64	5.39

Clear Creek Natural	100	5.60	5.60	5.60	0.27	0.03	2.00	5.29	2.79	5.57	36.35	7.50
Clear Creek Agricultural	40	5.44	5.44	5.44	-0.42	-1.15	-0.12	5.35	5.07	6.19	7.90	3.08
Slavkov Forest CZO	20	2.75	2.75	2.75	0.72	-0.97	0.93	1.98	1.81	2.78	24.08	3.22
Marchfeld CZO Initial Forest	200	0.22	0.22	0.22	0.04	0.04	0.04	0.18	0.08	0.29	17.48	6.01
Marchfeld CZO Grassland	“	0.15	0.15	0.15	0.07	0.05	0.09	0.08	0.06	0.09	28.16	6.79
Marchfeld CZO Cropland	“	0.21	0.21	0.21	-0.04	-1.03	0.01	0.24	0.19	1.23	32.56	13.22
Damma Glacier CZO - Young Soils	14	0.07	0.07	0.07	0.03	0.02	0.03	0.04	0.02	0.04	3.86	36.56
Damma Glacier CZO - Intermediate Soils	44	0.72	0.10	1.80	0.31	0.03	0.82	0.4	0.04	1.11	4.72	12.40
Damma Glacier CZO - Old soils	40	1.12	0.20	2.00	0.24	-0.10	0.60	0.81	0.28	1.45	12.11	14.08

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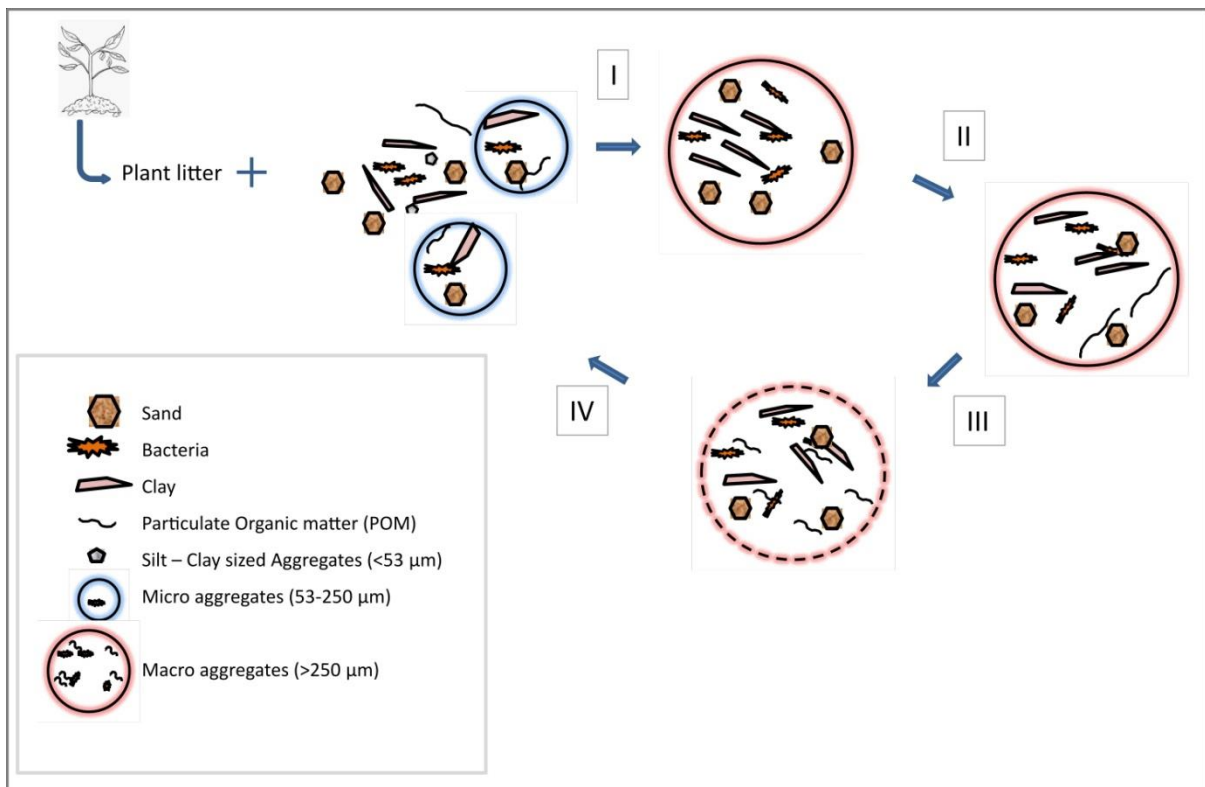
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716 **Figures**



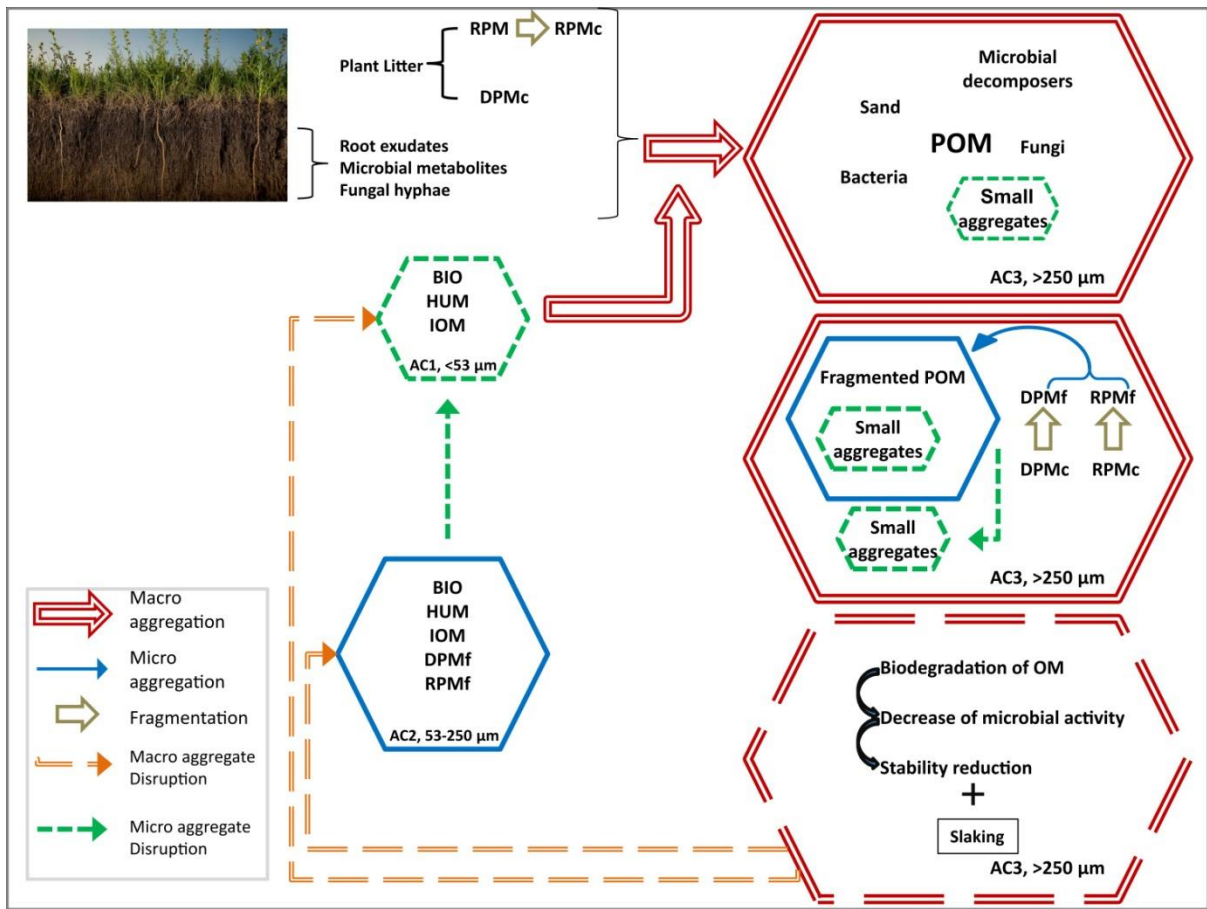
717

718 **Figure 1**



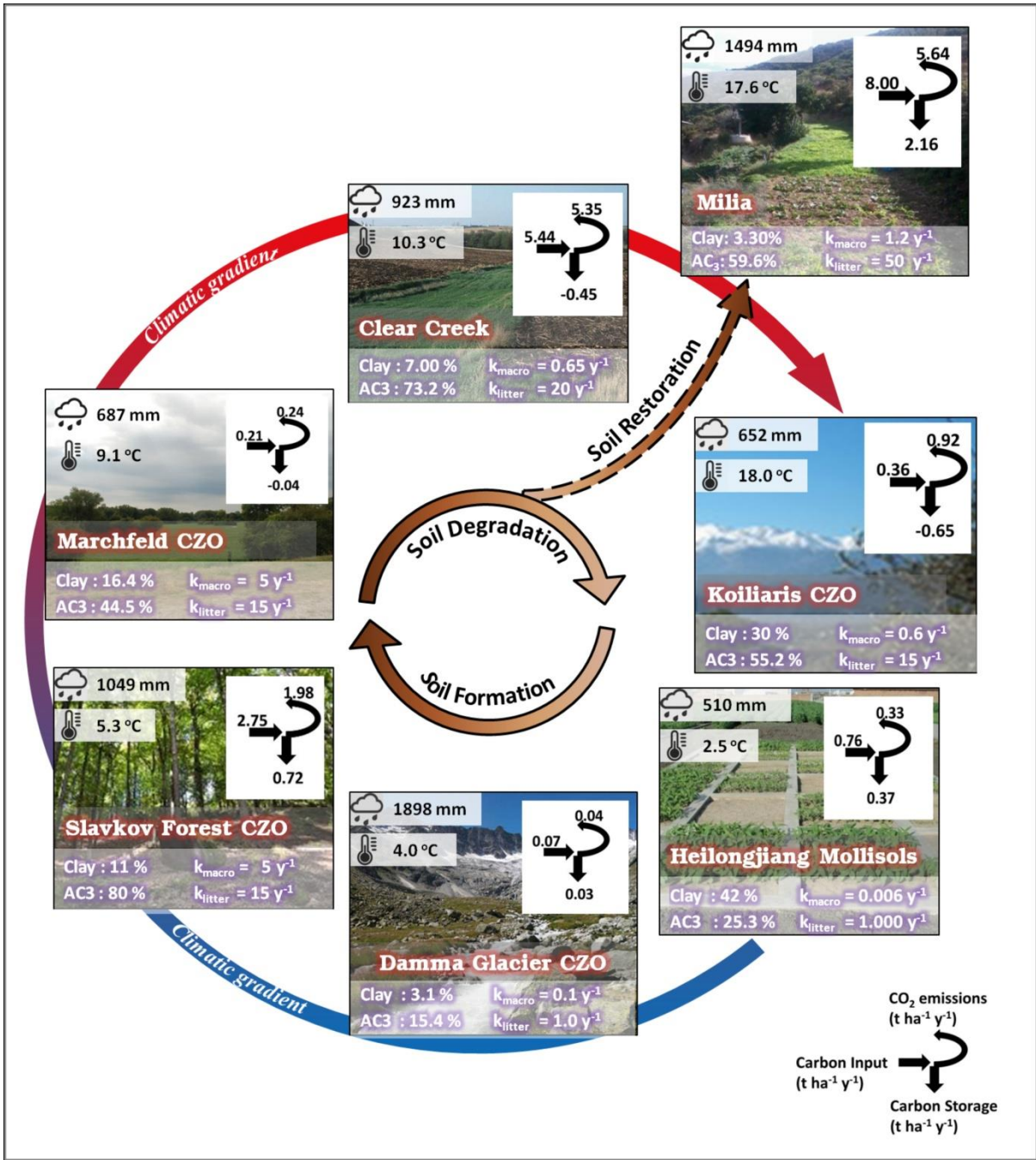
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720 Figure 2



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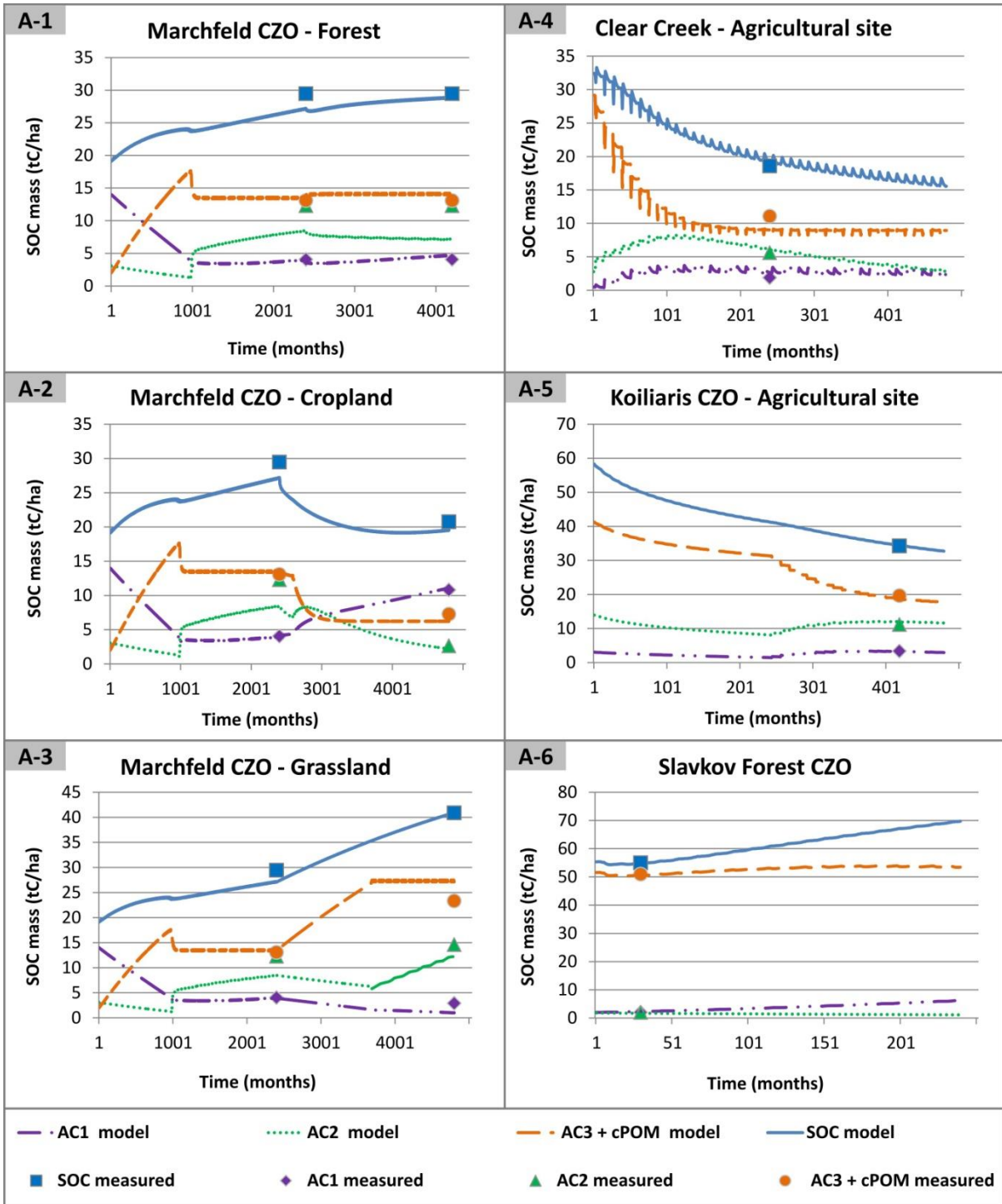
722 Figure 3



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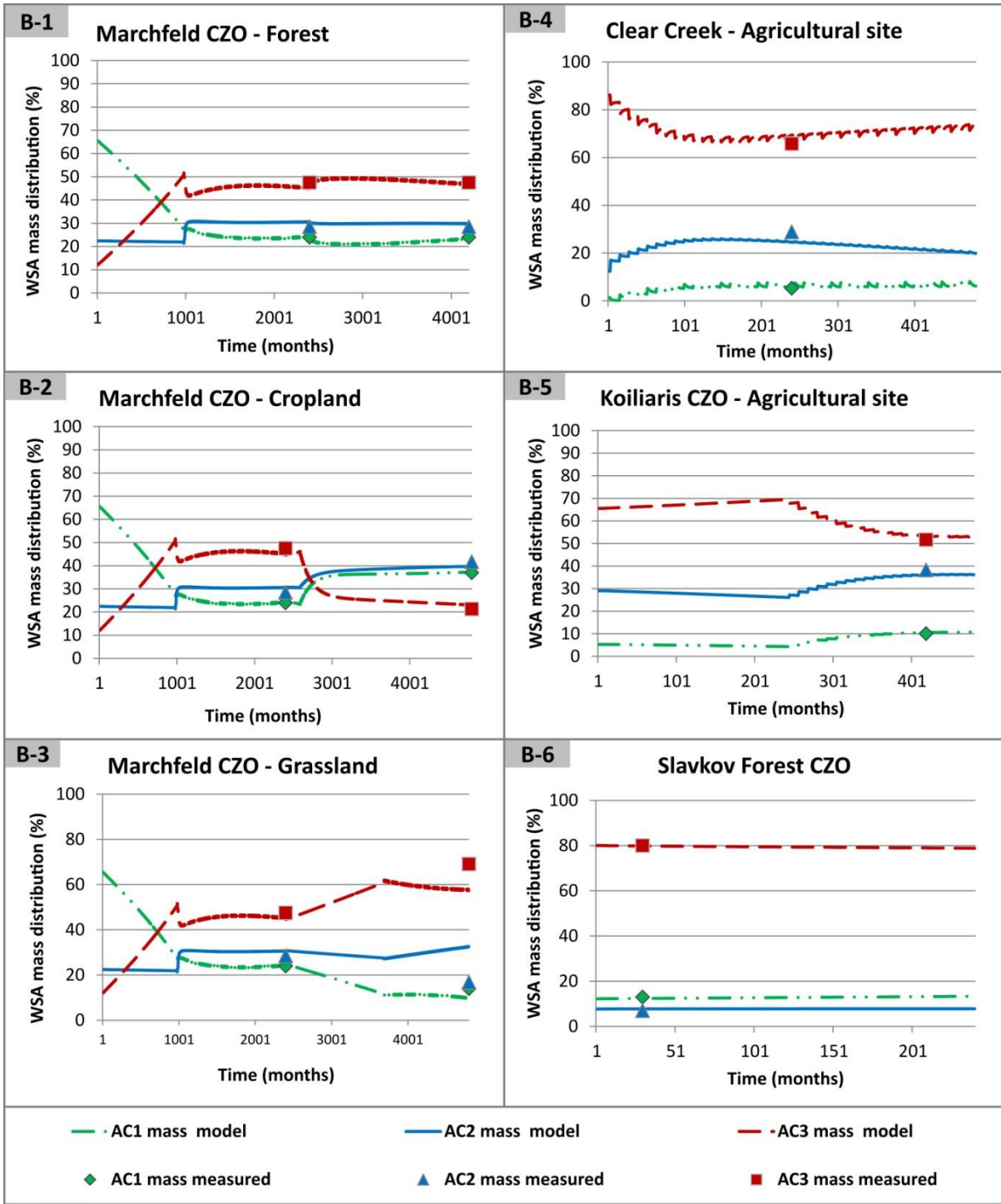
724 Figure 4





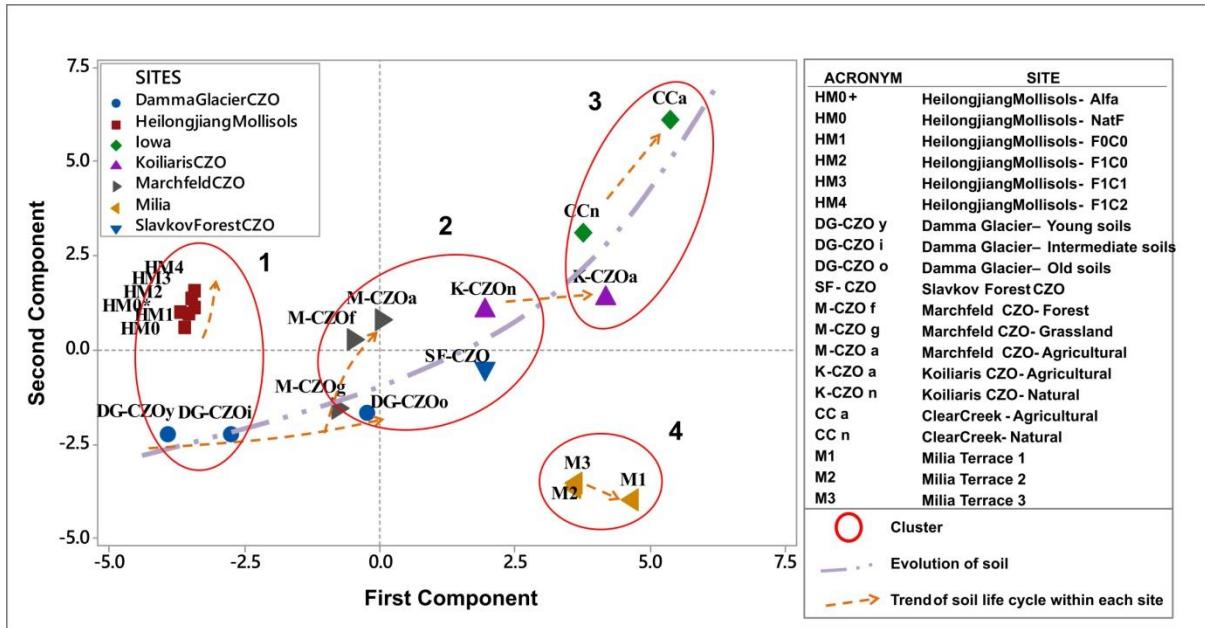
725

726 Figure 5a



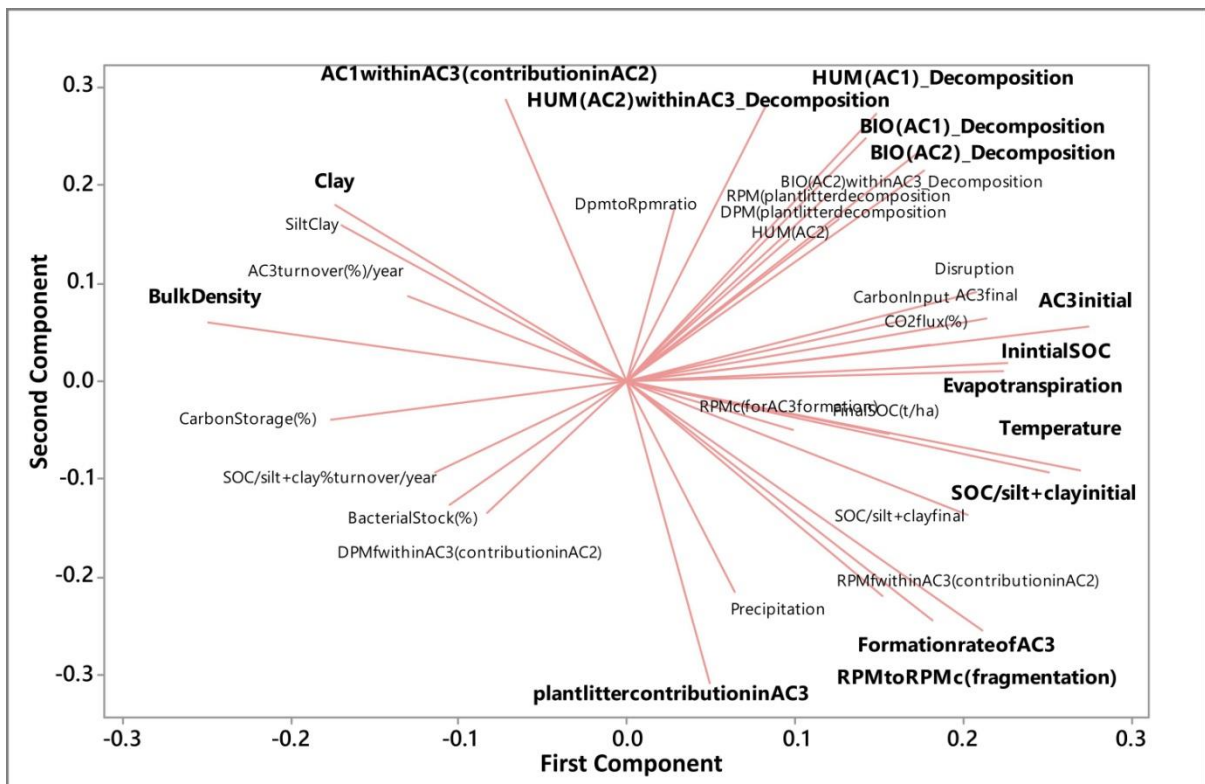
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728 Figure 5b



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730 Figure 6



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732 Figure 7

733 **Figure Legends**

734 Figure 1: Geographic distribution of the seven simulated sites (Google Earth, 2016)

735 Figure 2: Schematic representation of WSA formation modified from Stamati et al. (2013). The

736 particulate components that make up aggregates are not drawn to relative scale of their physical  
737 size.

738 Figure 3: Schematic representation of aggregation process, aggregate fractions and C pools included  
739 in the CAST model. The 3 large hexagons representing the AC1 macro-aggregate pool show in  
740 sequence, from top to bottom, 3 stages of macro-aggregate transformation from initial POM  
741 entering the soil, until it is decomposed resulting in breakup and release of AC2 and AC3  
742 aggregate fractions.

743 Figure 4: Study sites placed on a temperature gradient representing different stages of soil evolution  
744 from soil formation to soil degradation, including soil restoration. The ordering of sites  
745 according to soil formation/degradation pathway also coincided with the temperature gradient.

746 Figure 5a: Calibration results of Koiliaris CZO (agricultural), Clear Creek (agricultural), Marchfeld  
747 CZO (all managements) and Slavkov Forest simulations for the SOC stock distribution together  
748 with the field (measured) data used for the calibration. Regarding the goodness of fit of the  
749 calibration of the model, the mean RMSE for the SOC is 0.55, which corresponds to 0.55 t C/ha  
750 for the SOC stock distribution in a range of 1.03 to 55 t C/ha

751 Figure 5b: Calibration results of Koiliaris CZO (agricultural), Clear Creek (agricultural), Marchfeld  
752 CZO (all managements) and Slavkov Forest simulations for the WSA distribution together with  
753 the field data used for the calibration. Regarding the goodness of fit of the calibration of the  
754 model, the mean RMSE for the WSA is 1.29

755 Figure 6: Score plot of the components PC1 and PC2 of the Principal Component Analysis

756 Figure 7: Loading Plot of the components PC1 and PC2 of the Principal Component Analysis