

Accounting for soil architecture and microbial dynamics in microscale models: Current practices in soil science and the path ahead

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Abstract

Macroscopic models of soil organic matter (SOM) turnover have faced difficulties in reproducing SOM dynamics or in predicting the spatial distribution of carbon stocks. These models are based on a largely inadequate linear response of soil microorganisms to bulk concentrations of nutrients and it is clear that a new approach to SOM modeling is required. Introducing explicit microbial activity and OM reactivity in macroscopic models represents a challenge because of the fine spatial scales at which the processes occur. To get a better grasp on interactions that take place at the micro-scale, a new generation of SOM models have been developed at the spatial scale of the soil micro-environments where microorganisms evolve. They are well adapted to challenge traditional hypotheses about the

influence of soil architecture on soil microbial activity. Soil architecture provides the scene for a dynamic spatial accessibility of resources to microbes and the emergence of interactions between the actors of SOM decomposition. In this context, we review microscale models of microbial activity that have been designed for soils and soil analogs. To understand how these models account for spatial accessibility, we have looked in detail at how soil micro-environments are described in the different approaches and how microbial colonies are spatialized in these micro-environments. We present the advantages and disadvantages of the developed strategies and we discuss their limits.

Keywords: bacteria models, fungi models, microbial dynamics, microscale models, soil architecture, soil micro-environments, soil organic matter decomposition

Highlights:

- We review the state of the art in the development of microscale models of soil microbial processes
- Microscale models have integrated the tremendous progress in knowledge of OM cycling in soils
- We categorize modeling approaches in how they deal with complexity of soil architecture
- Modeling benchmarks are required to properly balance complexity and data uncertainty

1.Introduction

Over the last few years, a significant body of research has been devoted to improving the macroscopic models of the turnover of SOM that are integrated in large-scale C-cycling or climatic

44 models of the Earth. To try to account for sub-macroscopic heterogeneity, these macroscopic SOM
45 turnover models make use of empirical coefficients that are introduced to constrain turnover constants
46 as a function of soil water content and, in rare cases, of physical separation between OM and microbes.
47 In general, these tuning coefficients appear to provide sufficient degree of freedom to reach good
48 estimates of turnover dynamics under stable pedoclimatic situations. However, these models tend to
49 fail in transient situations, e.g., in response to increases in nitrogen fertilization or soil temperature
50 (Sierra et al., 2012). A common overall assessment is that these models are not capable of predicting
51 SOM dynamics accurately (Davidson et al., 2012; Sulman et al., 2018).

52 As a result, the assumptions embodied in these models have become increasingly challenged in
53 recent years. Various authors have argued that the idea of splitting SOM into distinct pools based only
54 on chemical composition and degree of recalcitrance no longer corresponds to the latest picture
55 available of the nature of SOM (Abramoff et al., 2018; Basile-Doelsch et al., 2020; Blankinship et al.,
56 2018; Dungait et al., 2012; Sainte-Marie et al., 2021 ; Yang et al., 2021). Among the pieces of evidence
57 that led to this perspective, Kleber et al. (2011) showed that the oldest SOM contains a greater
58 proportion of easily decomposable organic molecules, while the younger one contains organic
59 structures that are supposed to be more stable, suggesting that “C age is not necessarily related to
60 molecular structure or thermodynamic stability”. Other factors may explain the failure of macroscopic
61 models to predict SOM turnover. Among them, are the physical protection of SOM through
62 associations with poorly crystalline minerals (Kleber et al., 2005; Basile-Doelsch et al., 2020) and
63 carbon saturation controlled by organo-mineral interactions (Kleber et al., 2007). Another avenue that
64 has been explored to improve macroscopic models consists of accounting for microbial growth
65 explicitly (Wieder et al., 2015) in order to better predict the transient behavior of carbon fluxes during

66 environmental changes (Hadas et al., 1998 ; Lawrence et al., 2009 ; Sainte-Marie et al., 2021 ; Woolf
67 and Lehmann, 2019).

68 Another possible explanation for the failure of simple macroscopic models to describe the transient
69 dynamics of carbon and nitrogen fluxes in soils is that these models, from the start, are missing crucial
70 aspects of the functioning of soils. This perspective is in line with the conclusion, reached by
71 microbiologists sixty years ago, that microbial processes in soils are strongly influenced by the physical
72 and chemical properties of microenvironments in which microorganisms reside. Alexander (1965), in
73 particular, opined that without somehow taking into account the microscale heterogeneity of soils and
74 the characteristics of these microenvironments, now also referred to as hotspots (Kuzakov and
75 Blagodatskaya, 2015), it would be impossible to describe accurately the multivarious microbial
76 processes occurring in soils. This opinion has been confirmed by later experiments (e.g., Parkin, 1987),
77 and essentially the same message has been reiterated by Young and Crawford (2004).

78 In the last fifteen years, it has become increasingly acknowledged that the spatially heterogeneous
79 architecture of soil, the uneven distribution of water and air in the soil pores, and the heterogeneous
80 spatial distribution of trophic resources and microorganisms contribute to the emergence of microbial
81 processes in soils that cannot be accounted for solely with the macroscopic measurements that are
82 currently carried out (Baveye et al., 2018; Heitkötter & Marschner, 2018; Joergensen & Wichern,
83 2018). During the same time frame, it has also become increasingly clear that the static picture of
84 microorganisms confined to isolation in discrete microenvironments is inaccurate because
85 microorganisms are able to move in order to find their sustenance (e.g., Berg & Brown, 1972; Juyal et
86 al., 2018; Lacal et al., 2011; Kohlmeier et al., 2005; van Loosdrecht et al., 1990).

87 To our knowledge, Kuka et al. (2007) were the first to have attempted the development of a model
88 of SOM dynamics that accounts for the influence of pore space distribution. However, their model did

89 not account for positional relationships between the different classes of pores. Although model
90 predictions match remarkably a set of observations in an independent field trial, the parameterization of
91 fluxes necessarily lumps together the interactions between microorganisms and trophic resources, their
92 spatial disconnection, and the role of diffusion and/or advection between the different classes of pores.
93 To avoid this lumping together a new generation of SOM decomposition models has been developed
94 subsequently, accounting for the three-dimensional architecture of soil and the heterogeneity of the
95 distributions of microorganisms, water, air, SOM and reactive surfaces at the level of microbial habitats
96 (Baveye et al., 2018). In two recent mini-reviews, König et al. (2020) reported on microscale models
97 with a special focus on spatiotemporal dynamics of bacteria and bacterial functions in soil
98 microhabitats, and Golparvar et al. (2021) reported on microscale models of reactive transport
99 modeling in porous media.

100 In this general context, the key objective of the present review article is to assess the current
101 practices for considering soil architecture and microbial dynamics in microscale models of soil
102 microbial processes. We encompass models aimed at predicting SOM decomposition and greenhouse
103 gases emission, but also models whose aim is to better understand ecological interactions between
104 microbes as well as the emergence of the spatial organization of microbial colonies (bacteria and fungi)
105 and biodiversity. Indeed, these studies participate to the general understanding of SOM turnover since
106 for instance production of enzymes that are key factor in the depolymerization step of large polymers is
107 dependent on ecological and spatial interactions and biodiversity. Although not related to SOM
108 turnover, we also report some studies dealing with biofilm growth in artificial porous media for their
109 advanced understanding of the interactions between bacteria cycle of life and water flow. We focus on
110 i) the main modeling strategies to describe soil architecture according to a complexity gradient in
111 capturing the spatial heterogeneity at the scale of microhabitats (Section 2), and on ii) the main

112 strategies adopted to describe soil microbial dynamics, including that of soil fungi (Section 3). Then,
113 we discuss the advantages and disadvantages of these various strategies in Section 4. We address two
114 major limitations of efforts in this area to date, and discuss critically several options that could be
115 explored to fill knowledge gaps in the modeling of soil microbial functions (Section 5).

116

117 **2. Main modeling strategies to describe soil architecture at the microbial habitat** 118 **scale**

119 To review how the soil micro-environments are considered in modeling efforts, it is convenient to
120 classify the microscale models according to two criteria (Figure 1): i) the nature of the attributes of the
121 grid nodes, and ii) the degree of complexity of the description of soil architecture. From the point of
122 view adopted in this review, microscale models are classified as *implicit* when the node attributes
123 consist of bulk soil averaged variables: porosity, water content, and effective diffusion coefficients. By
124 contrast, microscale models are classified as *explicit*, also called “pore-scale” models, when the
125 attributes are Boolean values associated with only one phase, i.e., water, air, or solid, and, for the
126 former two phases, the diffusion coefficients are set equal to the corresponding molecular diffusion
127 coefficients in water or air. Implicit models only allow a simplified description of soil architecture
128 (Section 2.1), whereas the explicit strategy makes it feasible to reproduce actual, detailed soil
129 architectures as well as generate idealized soil architectures (Section 2.2). A mixed strategy considering
130 both implicit and explicit attributes is also sometimes adopted to describe detailed soil architectures
131 (Section 2.3). For each of these distinct approaches, we report how models account for the abiotic
132 processes that distribute air and water in the pore space, or lead to the transport of solutes (dissolved
133 organic carbon (DOC), NO_3^- , O_2 , etc) and gaseous products (CO_2 , CH_4 , N_2O), as well as the spread of

134 reactive solutes on soil solid surfaces. Finally, we report how solid and dissolved SOM and
135 microorganisms are spatially located in the soil architecture (Section 2.4).

136 Some of the studies cited in this review sometimes use the same model, either identically the same,
137 or a slightly modified (simpler or more complex) version of it. The technical description of the models,
138 their equations, and the parameters involved, are not always detailed enough to determine precisely
139 where the differences reside. We therefore decided to present this analysis considering each literature
140 source as an independent study.

141

142 **2.1 Implicit microscale models**

143 This strategy maintains the classical macroscopic approach, but it is applied at the level of
144 microhabitats. The micro-environments are spatially discretized in a regular grid and the size of the
145 grid nodes ranges from about $1\ \mu\text{m}^3$, i.e., roughly the average size of bacterial cells in soils, to about a
146 few mm^3 (Table S1). This strategy is adopted in 25 out of the 78 studies reported on this review.

147 Ignoring totally the underlying soil architecture and diffusion processes, Masse et al. (2007) and
148 Nunan et al. (2020) only distributed spherical spots of OM and of microorganisms in a 3D volume.
149 Then, based on population ecology, the models rely on physical contacts between microbial spots and
150 OM spots to achieve consumption and growth. To account for the spatial heterogeneity of the soil and
151 the variable accessibility of the resource for the microbial decomposers, the size of the microbial spots
152 can be varied (Garnier et al., 2008 ; Nunan et al., 2020).

153 Using a different approach, Folse & Allison (2012) model in a pseudo-2D grid the cooperation,
154 competition, and formation of coalitions in a community of enzyme-producing microbes. Nutrients
155 (carbon, nitrogen, and phosphorus) are unlimited and do not diffuse, whereas enzymes produced by

156 microorganisms diffuse. Each node of the grid lacks information on its nature (pore or solid), or on its
157 water and air content. All this information is encapsulated in a single effective diffusion coefficient of
158 the soluble substrates. Other studies on the emergence of a spatial structure of bacterial colonies repeat
159 this same approach (Kaiser et al., 2014, 2015; König et al., 2017, 2018, 2019; Wang & Allison, 2019).
160 In two other similar studies (Chakrawal et al., 2020; Pagel et al. 2020), the effective diffusion
161 coefficients are calculated via the macroscopic relationship proposed by Millington & Quirk (1961),
162 which considers hydration. However, spatial information about the water content at each grid node is
163 not provided.

164 This particular aspect is addressed by Evans et al. (2016), who simulate variably saturated
165 conditions to reproduce the Birch effect. However, soil water content is kept constant across all nodes
166 of the grid. Knudsen et al. (2006) develop a 3D model of hyphal growth under similar conditions.
167 Prescribed values for water content, nutrient availability, and temperature are attributed to each grid
168 node. However, like Evans et al., (2016), Knudsen et al. (2006) do not allow these attributes to vary
169 spatially. Thus, although these approaches go a step further to include spatial heterogeneity of
170 hydration conditions in the simulated domain, neither explores this potential. This further step is taken
171 in models studying the coexistence of competitive species under wet-dry cycles (Long & Or, 2005,
172 2009, Šťovíček et al., 2017). Long & Or (2005, 2009) vary the porosity and water content attributes
173 spatially over their grid node according to a log-normal distribution of the variances of the parameters
174 of the water retention curve proposed by van Genuchten (1980). Later, to describe more complex
175 ecological interactions (competition and mutualism), Kim & Or (2016) calculate the water content of
176 each node with the help of a fractal dimension to describe the roughness of the porous surface and
177 assume that pores have a conical geometry.

178 In the majority of implicit microscale models, physico-chemical processes are not considered at all.
179 In the few articles that are exceptions (Babey et al., 2017; Banitz et al., 2015; Gras et al., 2010, 2011;
180 Pagel et al., 2020), the sorption of dissolved OM components, organic pollutant (pesticide), and/or
181 NH_4^+ are described as mass transfer processes.

182

183 **2.2 Explicit microscale models**

184 **2.2.1 Case of detailed actual soil architecture**

185 The description of soil architecture generally relies on cutting-edge imaging techniques (e.g.,
186 Baveye et al., 2018; Lucas et al., 2020), such as through the use of X-ray computed tomography (CT),
187 either at synchrotron facilities or using table-top laboratory equipment. The quality and resolution of
188 the images determines the extent to which they may provide 3D spatial information about, e.g., the
189 geometry of the pore space, or of water and air interfaces, and about the location of solid particulate
190 organic matter (POM). Segmentation of CT images (e.g., Hapca et al., 2013; Houston et al., 2013;
191 Schlüter et al., 2014) is usually carried out in order to assign to each voxel one of the phases of the soil:
192 void or solid, with voids filled with water or air, solid being OM, minerals or matrix.

193 Of the 78 references reported in this review, only 9 studies encompass the actual architecture of
194 soils, using CT soil images as direct input data (Table S1). Attempts to model fungal growth have
195 considered the architecture of both repacked soil samples (Falconer et al., 2007, 2015; Pajor et al.,
196 2010) and undisturbed soil samples (Cazelles et al., 2013; Falconer et al., 2012; Kravchenko et al.,
197 2011;), whereas two studies on SOM decomposition by bacteria have used CT information obtained in
198 undisturbed soil samples (Portell et al., 2018; Vogel et al., 2015, 2018).

199 Measurements of air-water interfaces in soil using Synchrotron CT are available under very specific
200 conditions (e.g., Brusseau et al., 2007; Pot et al., 2015). However, models based on an actual soil
201 architecture so far have described unsaturated conditions via a mechanistic approach using a two-phase
202 lattice-Boltzmann model (LBM) that considers Van der Waals forces (Shan & Chen, 1993, 1994) and
203 capillary forces (Raiskinmäki et al., 2000). Phase separation simulations under static conditions
204 (Appert et al., 1991) can be performed for different water saturation conditions following the approach
205 proposed by Genty & Pot (2013). A 3D map of a continuous LBM fluid density is obtained, the highest
206 and the lowest densities of which can be associated to the water and air phases respectively (Portell et
207 al., 2018 ;Vogel et al., 2015). Then the soluble carbon substrate diffuses only in the nodes filled with
208 water according to the molecular diffusion coefficient of the substrate in water. The coefficient
209 according to which a fungal colony is assumed to diffuse through soil pores is maximal in the case of
210 lowest density (Falconer et al., 2012).

211

212 **2.2.2. Case of simplified actual soil architecture**

213 The models described in the previous subsection rely on a huge amount of information contained in
214 soil images, which is constantly increasing due to steady improvements of imaging techniques. Today,
215 3D CT images that are routinely acquired require several tens of gigabytes of storage for a size of up to
216 about 2000^3 voxels (Helliwell et al 2019; Koebernick et al., 2017; Quigley et al., 2018; San Jose
217 Martinez et al., 2018). The numerical solvers of the pore-scale models that directly include CT images
218 as input data, such as LBM or finite volume resolutions, require large computational and memory
219 capabilities. Thus, a more efficient strategy in terms of computer usage consists of reducing the
220 information amount by simplifying soil architecture. Two directions have been adopted to that end
221 (Figure 1). Either models retain the salient connectivity and size features of the pore space morphology

222 using morphological or irregular pore network models, or they generate grids or pore networks that
223 reproduce the statistical properties of actual soil samples as given by soil bulk measurements like
224 particle size distribution or percolation experiments. The studies adopting this strategy, 18 out of the 78
225 references, are reported in increasing order of simplification of soil architecture.

226 Morphological models are based on paving the pore space with an ensemble of simplified
227 geometrical primitives (usually balls, e.g., Vogel et al., 2005). This is done after having detected the
228 median axes of the pore space. Only the minimal set of maximal balls that make a piecewise
229 approximation of the pore space is retained (e.g., Al-Kharusi & Blunt 2007; Monga et al., 2007; Silin
230 & Patzek, 2006). This set constitutes the nodes of an adjacency graph considering the neighborhood
231 information of each ball or node where the decomposition of OM is calculated (Monga et al., 2008,
232 2009, 2014; Ngom et al., 2011). This ensemble is much more compact in terms of numerical data than
233 all the voxels of the CT image. Other 3D geometric primitives such as ellipsoids and generalized
234 cylinders (Ngom et al., 2012; Kemgue et al., 2019) have also been proposed, however they have not yet
235 been used to simulate SOM decomposition. In this strategy, unsaturated conditions are modeled using
236 the Young-Laplace law. The geometric primitives whose size does not exceed the size that would be
237 expected to drain at a prescribed water potential are filled with water leading to an explicit 3D
238 distribution of water and air at the nodes of the graph (Pot et al., 2015). The soluble carbon substrate
239 diffuses only in the water-filled nodes according to the molecular diffusion coefficient of the substrate
240 in water (Monga et al., 2014).

241 Irregular pore-network (PN) models are another valuable alternative to reduce the amount of
242 information contained in the soil images to a more manageable size. These models consist of an
243 ensemble of nodes connected to each other by links whose length, radius and number can be varied
244 (Blunt 2001; Xiong et al., 2016). The generated networks also keep most of the characteristics of the

245 pore space morphology: the pore size distribution, a mean degree of pore branching or connectivity
246 (e.g., Vogel & Roth, 2001), and the spatial heterogeneity of the clustering of pores and connectivity
247 (e.g., Blunt et al., 2002). While these irregular PN models are often used nowadays in computer fluid
248 mechanics (e.g., Martínez-Mendoza et al., 2019), the model of Perez-Reche et al. (2012) is the only one
249 that takes advantage of the potential of this approach to simulate microbial invasion in soils.

250 Simpler PN models based on a regular arrangement of the nodes are more often used, e.g., face-
251 centered cubic grids that retain only the pore size distribution and the mean degree of pore branching of
252 a soil. To simulate growth in cases involving a single bacterial cluster to several aerobic and anaerobic
253 communities, Ebrahimi & Or (2014, 2015, 2016, 2017, 2018) generate 3D regular angular PNs where
254 the coordination number of the nodes, the size distribution of the links and the porosity are defined
255 according to natural soil systems values or fitted in order to recover the van Genuchten (1980) water
256 retention curve parameters of a given soil (Table S1). The width and spanning angle of triangular links
257 can also be calibrated to soil water retention curves (Rosenzweig et al., 2013, 2014). This strategy is
258 much less representative of soil architecture than the approaches using irregular PN models or
259 morphological models, as noted by Blunt et al. (2002) and Ebrahimi et al. (2013). However, since
260 regular PNs do not describe the spatial arrangement of pores, some links can be randomly removed to
261 create spatial heterogeneity (Ebrahimi & Or, 2014). The length of the links can be changed to account
262 for tortuosity using helical bonds (Ebrahimi & Or, 2016). As with morphological models, the Young-
263 Laplace law is used to explicitly distribute water and air in the PN. The choice of a triangular cross-
264 section of the links makes it possible to more realistically simulate variable water contents than would
265 be possible if the links were spherical or cylindrical. In the latter cases, the application of the Young-
266 Laplace law leads to a binary response (empty or water-filled) and can thus promote greater
267 fragmentation of the liquid phase.

268 The flexibility of the latter approach permits also to generate multi-scale porous systems. Taking
269 advantage of a commercially available and widely used PN simulator (Xpore), and its predecessor
270 (Pore-cor), Laudone et al. (2011) develop a dual-porosity PN model. The positional relationships of the
271 macroporosity and microporosity are generated in order to fit several fundamental properties of soil,
272 namely water retention, aggregate size distribution, porosity of the microporous and macroporous
273 zones, and percolation characteristics (Laudone et al., 2013; Matthews et al., 2006). We observe that it
274 is also one of the few models that consider diffusion of gases (CO_2 , N_2O and N_2) emitted within the
275 pore space.

276 Finally soil architecture can be described by using a regular grid whose node attributes are
277 associated to pore or solid phases on the basis of statistical estimates of the pore sizes derived from a
278 set of published CT images of soil aggregates (Resat et al., 2012). However, in this approach, the actual
279 arrangement of pores is lost as pores are randomly placed on the grid with an additional constraint that
280 pores be continuously connected. Initial random assignment of nodes into pore and solid phases are
281 also considered in two pore-scale models that simulate temporal modifications of soil architecture
282 under microbial activity. Over time, solid nodes with a weak structure are spatially rearranged to
283 maximize the overall stability of solid node clusters (Crawford et al., 2012; Ray et al., 2017). This
284 stability is defined according to the local rate of production of stabilizing agents, whose concentration
285 is a function of the local respiration rate.

286

287 **2.2.3. Case of idealized soil architecture**

288 Columns filled with glass beads have occasionally been used to physically mimic soil architectures.
289 To describe these artificial packings, imaging (Graf von der Schulenburg et al., 2009; Peszynska et al.,
290 2016; Pintelon et al., 2012) or 2D mathematical algorithms of grain arrangement (Kapellos et al., 2007)

291 can be used as input data. With such algorithms it is also easy to introduce spatial heterogeneity, such
292 as the occurrence of fractures (Tartakovsky et al., 2009). A regular PN has also been generated based on
293 pore size distribution of a column packed with glass beads (Gharasoo et al., 2012, 2014). These
294 geometries are mostly used to study the permeability reduction due to the accumulation of biomass and
295 its metabolic by-products in coarse-textured porous media under water-saturated conditions. Water
296 flow, advection, and reaction-diffusion of soluble substrate are thus key processes in addition to
297 biological processes. To consider the higher viscosity of the biomass and associated exopolymers
298 compared to that of water, the coefficient of diffusion of the solutes through it can be reduced
299 compared to that in water (e.g., Tang et al., 2013).

300 To create synthetic rough, porous surfaces, 2D regular PN models with triangular channels are
301 generated based on typical pore sizes and connectivity. Variable water-saturated conditions can be
302 calculated with the Young-Laplace law. This approach has been adopted to model the motility of
303 bacteria and expansion of bacterial colonies (Wang & Or 2010), as well as the coexistence (Borer et al.,
304 2018 ; Long & Or 2007; Wang & Or 2012, 2013) and self-organization (Wang & Or, 2014) of bacteria.
305 Wang & Or (2012, 2013), simplify the time-consuming explicit calculation of solute diffusion-reaction
306 processes in the links of the PN by directly calculating an effective diffusion coefficient at each node
307 using the Millington & Quirk (1961) expression using the node water status as input. This
308 simplification brings this contribution closer to an implicit description of soil architecture (see Section
309 2.1).

310 Random assignment of pore and solid nodes is also commonly used to generate soil analogs.
311 Falconer et al. (2008) create porous media of porosity varying between 0 and 1 and simulate fungal
312 invasion. Other authors have considered instead a random assignment of collections of nodes made
313 impervious to mycelium and nutrient diffusion (Boswell et al., 2007; Boswell, 2008; Boswell &

314 Hopkins, 2009; Vidal-Diez de Ulzurrun et al., 2017). In a simpler form, the fungus models of Boswell
315 et al. (2003) and Boswell & Hopkins (2009) do not consider impermeable materials but a spatially
316 heterogeneous initial distribution of the carbon substrate in the form of different tessellations. In these
317 cases, diffusion of the substrate external to the fungus is not permitted.

318 Different sizes and lengths of geometrically highly simplified, linear pores in 2D are used to assess
319 the role of salient soil pore geometry, from shallow pores to deep crevices with small opening, on the
320 growth and survival of bacteria (Resat et al., 2012). Using the COMSOL Multiphysics software applied
321 to a pore of uniform geometry, Schmidt et al. (2018) assess the influence of the spatial location of
322 bacterial colonies along the pore on the biodegradation of an organic substrate that moves through it.

323 Finally, experimental micro-models of diverse geometrical forms like a succession of rectangular
324 water-saturated microhabitats (Keymer et al., 2006), packing of cylinders, and etched-glass networks
325 (Borer et al., 2019) have been reproduced in a number of computational models (Borer et al., 2019;
326 Centler et al., 2011; Knutson et al., 2005; Tang et al., 2013). Due to simplification of the reproduced
327 micro-models into a 1D grid, Centler et al. (2011) use effective diffusion coefficients for the substrate
328 and bacteria, together with effective chemotactic sensitivity constants towards the substrate and the
329 bacteria.

330

331 **2.3 Mixed explicit/implicit microscale models**

332 A final strategy mixing implicit and explicit attributes of the grid nodes to describe actual soil
333 architecture from soil imaging is adopted in two studies (Yan et al., 2016, 2018). In this approach, a
334 dual threshold segmentation of the CT images is used to obtain ternary images where the gray voxels
335 whose value lies between the two thresholds that define voids and solids are associated with a mix of

336 pore and solid phases. These latter nodes have an implicit porosity attribute whose value depends on
337 the gray level scale (Figure 1). The diffusion coefficients of the dissolved OM, O₂ and CO₂ are equal to
338 their molecular diffusion coefficient in liquid and air phase for the explicit water and air voxels,
339 respectively. Whereas for the implicit unsaturated voxels, the diffusion coefficients are calculated
340 according to empirical laws (Archie, 1942; Hunt, 2004). Mixed explicit and implicit diffusion
341 coefficient attributes of the grid nodes are thus used in this approach. Additionally, the sorption
342 processes of OM are described by mass transfer rates using effective surface reactivity parameters.

343

344 **2.4 Spatial description of the initial distribution of SOM and microorganisms in the**

345 **reviewed models**

346 It is critical to consider how OM is distributed within the soil architecture. Although combined
347 staining and/or chemical and imaging techniques are promising tools (e.g., Maenhout et al., 2021; Peth
348 at al., 2014; Roose et al., 2016) they are far yet from routinely providing data. Therefore, the placement
349 of SOM has been mainly considered through modeling scenarios. When SOM consists of dissolved
350 nutrients, it is most of the time homogeneously applied at the nodes of the grid (e.g., König et al., 2018)
351 and/or applied at specific locations in the simulated domain to produce gradients or counter gradients
352 between carbon and O₂ (e.g., Ebrahimi & Or, 2015). Metabolites or enzymes produced by microbial
353 activity are located at the nodes of the producers (e.g., Folse & Allison, 2012), from where they diffuse.
354 When SOM consists of solid pieces, different distribution scenarios have been used ranging from
355 aggregated to dispersed distributions (e.g., Falconer et al., 2015). Likewise, microorganisms are either
356 homogeneously located in the simulated domain (e.g., Gharasoo et al., 2014), randomly distributed
357 (e.g., Portell et al., 2018), or locally placed (e.g., Ebrahimi and Or, 2015, Falconer et al., 2015;

358 Kravchenko et al., 2011), and the effect of different distributions can be explored. They can also be
359 placed according to the size of pores (e.g., Monga et al., 2009). Models using explicit attributes and
360 describing actual soil architectures tend to locate bacteria in water-filled nodes where they are assumed
361 to live (e.g., Vogel et al., 2015) while fungi preferentially invade air-filled nodes (e.g., Falconer et al.,
362 2012). Only one model (Pagel et al., 2020) uses different probabilistic distributions based on Raynaud
363 & Nunan (2014) who integrate data in the visualization of microorganisms in soils (Nunan et al., 2003).

364

365

366 **3. Main modeling strategies to describe the microbial dynamics in microscale** 367 **models**

368

369 In this section, we focus first on the nature of SOM pools, the type of microorganisms and the
370 strategies used to distribute them spatially in their microhabitats. Then we focus on biological
371 processes, encompassing substrate decomposition, microbial substrate uptake, microbial growth,
372 microbial metabolic processes and mobility. It would make sense to report the microbial dynamics
373 modeling approaches in terms of the soil spatial representation since the latter is at the heart of the
374 reported microscale models. However, the number and the degree of details of the biological processes
375 are not linked with the degree of representativeness of actual soil architecture or the choice of implicit
376 or explicit grid node attributes. Rather, it is the research question to which all these micromodels try to
377 answer that has dictated the strategy. This is evidenced in Table 1 which lists the references from the
378 most to the least accurate soil spatial representation. Table 1 provides details of each of the biological

379 processes, the nature of SOM pools, microorganisms and modeling strategy to describe
380 microorganisms colonies.

381

382 **3.1 Nature of substrates and microorganisms**

383 Most of the studies (51 out of the 78 references) consider a single simple soluble substrate
384 (monomer) that is directly taken up by microbes (Table S1, e.g., Long & Or, 2007). Other studies (24
385 references) consider a preliminary step of decomposition (depolymerization) of complex solid substrate
386 (polymers) into soluble organic compounds that are taken up by microbes (e.g., Pagel et al., 2020). Of
387 the 78 references, two studies do not specify the nature of microorganisms (Perez-Reche et al., 2012;
388 Crawford et al., 2012), and only 13 relate to filamentous fungi, while the others relate to bacteria,
389 including 9 references that deal with accumulation of bacterial biomass and associated exopolymers.
390 Bacteria models generally simulate a single specific species or strain (in 47 references, e.g., Knutson et
391 al., 2005), or up to eight different genotypes (Folse & Allison, 2012) or 10 different taxa (Nunan et al.,
392 2020). Fungi models simulate a single species except for Falconer et al. (2008) that are the only ones to
393 study more than one fungal species, comparing compatible and/or antagonist species. Most bacterial
394 models describe i) generic functional groups such as anaerobic bacteria, aerobes, methanogens (e.g.
395 Ebrahimi & Or, 2018), ii) generic competitive species such as competitive, generalists, or cheaters for
396 the same resource (e.g. Kaiser et al., 2014 ; Monga et al., 2008 ; Pagel et al., 2020) or from a range of
397 specialists of a single resource to generalists of up to ten different resources (Nunan et al., 2020). Three
398 studies consider commensal or mutualistic relations in microbial consortia. In their simplest form, the
399 models consider a chain of up to three substrates and microbe species, with one of the species
400 dependent on one substrate produced by other species (Wang & Or, 2014 ; Kim & Or, 2016). In its

401 most complex form, the model of Borer et al. (2019) which is based on the COMETS model of
402 Harcombe et al. (2014), encompasses a reduced metabolic network involving more than a hundred
403 metabolites and reactions.

404

405 **3.2 Modeling strategies to describe microbial colonies**

406 **3.2.1 Case of bacteria**

407 About a third of the references (21 out of 62 studies dealing with bacteria) model the life cycle
408 processes at the scale of bacterial colonies that are spatially distributed in the soil pore space. This
409 population-based strategy calculates the growth of a single (lumped) mass of bacteria representative of
410 the microorganisms contained in a given microhabitat. Cell division is not considered and mortality
411 processes (starvation or predation) are assumed to be continuous processes (e.g., Vogel et al., 2015).
412 The updating scheme is synchronous, i.e., uptake, growth, mortality occur at the same time for the
413 whole microcolony.

414 Another strategy, adopted by 37 references, models the life cycle processes at the scale of
415 individuals, which are the bacteria cells (e.g., Graf von der Schulenburg et al., 2009). In this individual-
416 based, or agent-based modeling approach (Hellweger & Bucci, 2009), cell division processes are
417 discrete events, a feature that facilitates the discretization of the spatial expansion of the population.
418 Starvation mortality or predation processes are discrete events (the whole cell dies, not a fraction of it).
419 In addition, interspecific and intraspecific variability in the individual properties are considered (e.g.,
420 size or mass threshold to start cell division). Synchronous updating (e.g., Kreft et al., 1998) or
421 asynchronous updating (e.g., Ginovart et al. 2005) schemes can be used. Despite the fact that, in the
422 presence of recycling processes, differences can appear between both schemes (Caron-Lormier et al.,

423 2008), the type of updating of individual-based models is not always stated, which complicates
424 reimplementation and, ultimately, reproducibility of the research.

425 Meta-agents, or “superindividuals”, i.e., ensembles of single bacterial cells, are used to mitigate the
426 large computation costs associated with the description of processes at the single-cell level (Banitz et
427 al., 2015; Borer et al., 2019; Masse et al., 2007). This coarse-grained description is also used by Long
428 & Or (2005) who adopt the random walker model developed by Ben-Jacob et al. (1994). Using this
429 approach, the question remains how to identify the size of the meta-agents that makes it possible to
430 retain the influence of the individual behavior of bacteria.

431

432 **3.2.2 Case of fungi**

433 The fungal “individuality” is much more difficult to define as compared to bacteria. Fungi are
434 multicellular organisms that spread in the pore space. Fungi grow as an interconnected network of
435 hyphae, named mycelium or fungal colony. The shape of the whole fungal colony thus needs to be
436 considered. None of the reviewed fungal models considers single cells. Continuous models and
437 individual-based models of fungal growth have been distinguished (Boswell & Hopkins, 2009, Table
438 S1). In the former approach, the fungal mycelium is considered as a continuous biomass (e.g., Boswell
439 et al., 2003; Falconer et al., 2007), whereas the individual-based approach considers individual hyphae
440 explicitly and describes the discrete (random) events involved when they grow and branch (e.g.,
441 Knudsen et al., 2006; Boswell et al., 2007).

442

443 **3.3 Description of biological processes**

444 **3.3.1 SOM hydrolysis**

445 In some models (e.g., Long & Or, 2005), the depolymerization step of SOM is assumed to be
446 independent of microbial growth and be described by a fixed hydrolysis rate. Often, models assume
447 that depolymerization depends on enzyme production (e.g., Allison, 2005) or microbial growth (e.g.,
448 Falconer et al., 2015). Complex biogeochemical reactions including mixed kinetics and thermodynamic
449 equilibrium reactions, such as oxic degradation of SOM (Aguilera et al., 2005), are calculated for the
450 soluble substrate, using the Biogeochemical Reaction Network Simulator in one study (Gharasoo et al.,
451 2012).

452 The mathematical description of SOM hydrolysis follows the three conceptual classes described by
453 Wutzler & Reichstein (2008), which represent respectively no-, linear- and non-linear dependencies on
454 decomposer biomass. In the first class, constant rates or more often Michaelis-Menten kinetics (e.g.,
455 Kaiser et al., 2014) are used. The latter permits an indirect dependence on biomass uptake and growth
456 through microorganisms that produce enzymes. Chakrawal et al. (2020) use the three conceptual
457 classes in a comparative study.

458

459 **3.3.2 Microbial substrate uptake and growth**

460 In its simpler form, and depending on the research question, growth of biomass is neglected (in six
461 references, e.g., Laudone et al., 2011; Crawford et al., 2012) and a constant biomass value is used. A
462 large number of studies (36 references) use the Monod equation to describe the non-linear growth of
463 decomposer biomass (e.g., Banitz et al., 2011) whereas linear kinetics is adopted in eight references
464 (e.g., Boswell, 2008; Gharasoo et al., 2014). The logistic growth is also described in two studies
465 (Centler et al., 2011; Gharasoo et al., 2014). Fixed rates are used to calculate growth in the six
466 references that adopt the offer-demand approach (e.g., Masse et al., 2007; Monga et al., 2008). In five
467 studies, growth is calculated from metabolic pathway reactions (e.g., Gras et al., 2011; Borer et al.,

2019). Finally, in one case, growth is implicitly modeled by increasing the size of the area where the cell consumes the resource assuming the increase to be an inverse function of the catabolic breadth of the cell taxon, i.e., the range of organic substrates that can be used (Nunan et al., 2020).

Microbial substrate uptake and growth can also be limited by the availability of other nutrients (N, P) and O₂. Two approaches are adopted. Either microbe stoichiometry constraint limits uptake (e.g., Allison, 2005) or the concentration of the limiting factor is introduced in the Monod formalism. In the latter case, the dual-Monod equation is generally used (e.g., Yan et al., 2016) or the minimum of the Monod equations established for each substrate (Borer et al., 2018; Kim & Or, 2016). In one reference, a multi-substrate Monod kinetics is used to describe the uptake of small polymers and monomers (Pagel et al., 2020).

3.3.3 Microbial metabolism

Almost two third of the references consider microbial maintenance (e.g., Boswell et al., 2003; Resat et al., 2012). Growth respiration is generally implicitly considered by using the assimilation yield, whereas more rarely it is integrated in a lumped respiration term that does not distinguish maintenance and growth respiration processes (e.g., Vogel et al., 2018). The production of metabolites by microorganisms can be directly calculated in the form of enzymes (e.g., Evans et al., 2016), by-products (Kim & Or, 2016), generic inhibitor (Falconer et al., 2008; Kravchenko et al., 2011) or sticky agents (Ray et al., 2017), which can undergo transformation (decay) or sorption processes.

The production of greenhouse gases is not always modeled (27 references), and when it is, the majority of studies deal only with CO₂ (e.g., Nguyen-Ngoc et al., 2013), whereas a minority also calculate denitrification and emission of N₂O (Ebrahimi & Or, 2015, 2016, 2018; Laudone et al., 2011) or CH₄ (Ebrahimi & Or, 2017, 2018).

491

492 **3.3.4 Microbial death, recycling, and dormancy**

493 Microbial decay processes are mostly described by starving death (48 references, e.g., Allison,
494 2005) and additionally by predation (e.g., Portell et al., 2018). However, only one reference explicitly
495 simulates predator growth (Pagel et al., 2020). The recycling of dead biomass in solid- (e.g., Gras et al.,
496 2010), soluble- (e.g., Wang & Allison, 2019), and in both solid and soluble forms (e.g., Folse &
497 Allison, 2012; Monga et al., 2014) appears in 17 references. Dormancy is only accounted for in 12
498 references (e.g., Resat et al., 2012).

499

500 **3.3.5 Microbial mobility**

501 Colonization is a key behaviour of fungi and it is driven by hyphae invasion. Advective and
502 diffusive movements including apical growth and branching (e.g., Boswell, 2008) or solely diffusive
503 movements (e.g., Falconer et al., 2007) are described. The hyphae segments can be constrained to grow
504 and branch on a regular lattice (Boswell, 2008 ; Boswell & Hopkins, 2009 ; Boswell et al. 2007) or the
505 geometrical constraint on orientation of hyphae growth can be relaxed when using a lattice-free
506 approach (Knudsen et al., 2006; Vidal-Diez de Ulzurrun et al., 2017). Fungal networks generated with
507 these lattice-free models are more realistic morphologically than the ones generated with the lattice-
508 based approach but they require much more computational resources (Boswell & Hopkins, 2009).

509 A large majority of the bacterial models account for movement. Motility can be considered as a
510 simple random motion from one node containing bacterial cells to a neighbor node (e.g., Ginovart et
511 al., 2005). The choice of the neighbor can be further constrained by hydration status (Long & Or, 2005,
512 2009) of the targeted node, its chemical nature (cellulose adhesion in Resat et al., 2012) or the size of
513 pore (Perez-Reche et al., 2012). Cell motion is described only during the cell division process (e.g.,

514 Kaiser et al., 2014) or in situations of excess biomass (e.g., Knutson et al., 2005 ; Graf von der
515 Schulenburg, 2009). Several studies have accounted for cell propulsion due to flagellated motility
516 where hydration status can reduce the cell velocity (e.g., Wang & Or, 2010), chemotaxis process toward
517 substrate (e.g., Ebrahimi & Or, 2015) or towards bacteria (e.g., König et al., 2017). Two studies (Banitz
518 et al. 2011, 2016) consider bacterial diffusion along analogs of fungal network hyphae, whereas others
519 account for the effect of shear stress which can reduce the movement of bacteria cells (e.g.,
520 Tartakovsky et al., 2009).

521

522 **3.3.6 Carbon translocation by fungi and anastomosis**

523 Carbon translocation along fungal mycelium is driven by the concentration gradients of the internal
524 substrate along the hyphae (e.g., Falconer et al., 2007) while an active translocation can additionally be
525 described (e.g., Boswell, 2008). Anastomosis is explicitly considered by removing hyphal tips when
526 they move to a node that already contains a hypha (e.g., Boswell, 2008). Hyphal interactions that can
527 result in the fusion of two individual colonies or maintain mycelial individuality of somatically
528 incompatible genotypes are described in Falconer et al. (2008).

529

530 **4. Discussion about the main modeling strategies**

531 **4.1 Soil architecture**

532 In all the reported studies, the inclusion of a spatial component is at the heart of the latest generation
533 of microscale models to make ecological interactions emerge and explain soil microbial activity. The
534 value of studies that use implicit approaches to summarize the environment is to emphasize the role of
535 space and dispersal in ecological interactions, which can lead to patterns and hotspots that would not be

536 observed in well-mixed system. The advantage of this approach is that these models rely on a few,
537 easily measured bulk soil variables (Table 1). However, they cannot establish new mechanistic
538 relationships between soil architecture descriptors and soil microbial response since they are dependent
539 on empirical macroscopic laws like those relating the effective diffusion coefficients to hydration.

540 At the opposite end of the spectrum, methods that use explicit attributes can obviously capture most
541 of the spatial heterogeneity of the clustering and connectivity of pores. This approach uses new
542 knowledge of the microscale intricacies of soil architecture, which until recently had remained a black
543 box for a long time. It offers the possibility to identify relevant 3D soil architecture descriptors that
544 explain soil microbial activity and *in fine* will help upscale microbe activity from the micro-scale to the
545 core-scale. The level of accuracy of the description of spatial heterogeneity needed in this approach has
546 opened the brought-together scientists of various and complementary fields (soil science, mathematics,
547 computer vision, ecologists, physicists). However, this strategy needs a huge amount of input data and,
548 as a consequence, simulations require tremendous computing calculations and memory operations,
549 which limits the size of the investigated domain that can be considered (Table 1). In the case of
550 idealized geometry, like those of experimental micromodels or packings of glass beads, explicit
551 attributes permits to exactly reproduce the geometry and helps validate the models (Table 1). The
552 disadvantage is that actual soil architecture cannot be investigated.

553 The value of the approaches that describe simplified actual soil architecture or idealized porous
554 media (which encompass regular grid and regular PN models) is to explore simplified scenarios of the
555 complexity of pore spatial arrangement to investigate its potential role in soil microbial response (Table
556 1). The great advantage of methods based on morphological or PN models is that once the simplified
557 networks have been defined, processes can be simulated much more efficiently allowing for larger
558 samples at greater speed to be tested. A disadvantage is that these methods tend to focus on single

559 aspects of the pore space such as connectivity, volume, pore-size distribution, but may not capture well
560 the pore-solid interface area, which is critical for many processes in soil. It is also not clear at this stage
561 whether regular PN are sufficient to catch the complexity of pore arrangement as compared to the more
562 realistic irregular PN. Indeed, it is far from certain that predicted key factors in SOM microbial
563 decomposition like accessibility between OM and decomposers is correctly captured in regular PN.
564 Furthermore, only a limited number of soil types has been sufficiently described to provide reliable
565 statistics on the pore space morphology. They are necessary data to generate regular PN, and this
566 renders quantification of the soil microbial activity by this approach very questionable.

567 We observe that the more realistic the description of the 3D soil architecture is, the more
568 mechanistic is the description of the distribution of water and air in the pore space, calculated from
569 physical laws that consider interfacial and capillary forces, giving rise to realistic air-water interfaces
570 (Table 1). It is surprising that none of the PN models reported in this review calculate mechanistically
571 the invasion of the air phase in pores as a function of the evaporation rate, as for example Yiotis et al.
572 (2001) did. They all rely on the empirical Young-Laplace relation, which is based on a cylindrical
573 representation of pore geometry. Finally, knowledge on the spatial location of microbes in soils (e.g.,
574 Eickhorst & Tippkötter, 2008 ; Nunan et al., 2003) has not been taken into account so far in microscale
575 models. At best, scenarios based on statistical models of spatial distribution of bacteria (Raynaud &
576 Nunan, 2014) have been used. Likewise, data on the spatial location of tiny SOM patches using
577 staining techniques (e.g., Peth et al., 2014) or multimodal data acquisition on spatial location of
578 chemical elements (Hapca et al., 2011) and bacteria (Schlüter et al., 2019) have not been used although
579 they can be easily implemented in approaches considering explicit description of soil architecture.

580

581 **4.2 Microbial dynamics**

582 Given the large variety of processes described no consensus seems to emerge on the optimum choice
583 of a spatial modeling strategy. Almost one third of the reported studies used population-based
584 approaches, and the choice of the approach was not related to the size of the grid node volumes that
585 could reach down to a few μm^3 (Table S1). At this scale, a limited number of individuals can be
586 contained in a node and this should in principle call for an individual-based approach rather than a
587 population-based one, meant to represent large numbers of microorganisms. Indeed, population-based
588 and individual-based model results will diverge when there is a low number of individuals, because in
589 this case, the randomness of discrete events can result in a behavior that is different from the average
590 (Boswell & Hopkins, 2009). This is particularly true when the microenvironments of soil microhabitats
591 are depleted in nutrients which would prevent the development of a large number of individuals.
592 Randomness of events, like motility used as a strategy to alleviate starving conditions, could make
593 emerge a different picture than in population-based models.. The same criticism could be levied to a
594 large extent toward individual-based microscale models, which still adopt the Monod equation to
595 describe bacterial growth, even though this usage of the equation for small groups of cells is not
596 warranted at all, and other formalisms exist (Bermúdez et al. 1989). Nevertheless, irrespective of the
597 modeling formalism used, encapsulating microbial growth at the single cell level allows to account for
598 interspecific and/or intraspecific variability as well as the influence of random effects, which can have
599 a high influence at low microbial numbers.

600 In this review we voluntarily omitted to report on numerical schemes used to solve the partial
601 differential equations (PDEs) describing biological as well as physical processes, adopting in this
602 respect the point of view that the methods used have been intensively verified and assessed by
603 numerical analysts(e.g., Ginzburg et al., 2008; Hecht, 2013) and it is not the purpose of this review to

604 evaluate them, in part because benchmarks have to be developed for microscale models simulating
605 microbial activity.

606 An encouraging finding is that microscale models have integrated the tremendous progress in
607 knowledge of OM cycling in soils. Even though the vast majority of models simulate the uptake of
608 simple monomers, when they take into account the solid form of SOM they all include a
609 depolymerization step to produce dissolved OM that is taken up by microorganisms. The description of
610 this process is generally less complex when actual soil architecture is considered, perhaps to keep the
611 overall complexity of the models within computationally manageable bounds, whereas more
612 complicated reactions of depolymerization are found when soil architecture is simplified or idealized.

613 Similarly, microscale models have attempted to integrate the knowledge gained on ecological
614 interactions between species. Even though the vast majority of models simulate a single species, when
615 they consider different species, they include ecological interactions between species from the simpler
616 case of competition for food to more complex interactions (mutualism or commensalism). Once again,
617 the simpler representations of ecological interactions tend to be adopted when actual soil architecture is
618 described. We also note that none of the microscale models have so far coupled fungi and bacteria
619 except the models of Kaiser et al. (2014) or Pagel et al. (2020), which do it through different
620 parameterizations of growth and uptake and not through different expansion rules. As fungi and
621 bacteria or archaea operate at different spatial scales (a fungal colony can translocate nutrients over
622 cm's), the combination of both in a single model is currently challenging and hampered by
623 computational limitations.

624 Most of the microscale models have also integrated some of the increasing knowledge about
625 microbial mobility in soil (e.g., Juyal et al., 2020). However, bacterial models that describe in detail the
626 complexity of soil architecture have tended to disregard this process. No consensus has been reached in

627 general on the type of motility that needs to be included in models, as random motion and/or
628 chemotaxis can be found in experiments, mostly depending on the research question being addressed.
629 Advanced descriptions of spatial distribution of soil microorganisms derived from ecological
630 knowledge have also started to be considered in the latest generation of microscale models (Pagel et al.,
631 2020).

632 Although tremendous progress has been made toward understanding the role of O₂ on microbial
633 activity (e.g., Keiluweit et al., 2016), few studies have integrated that knowledge. Most models
634 consider decomposition of SOM under optimal O₂ diffusion and do not describe O₂ diffusion in the
635 liquid phase. Similarly, although the role of air-filled pores in the emission of N₂O has been
636 demonstrated experimentally (e.g., Rabot et al., 2016), of the five microscale models that describe
637 denitrification processes, only one includes diffusion of the emitted gases (N₂ and N₂O) in the liquid
638 and gas phases within the soil. Whereas diffusion of the produced CH₄ is ignored at the pore-scale in
639 virtually all models, it is considered by one 1D-upscaled model at the scale of the soil profile (Ebrahimi
640 & Or, 2017).

641 Perhaps the most striking feature of existing models is the fact that the majority of them so far have
642 not accounted for the presence of roots, despite the rhizosphere being the most active region in soil.
643 Models simulating root surface colonization by bacteria have focused on the description of the root
644 itself and its growth while the rhizosphere is either considered as inactive grid nodes, in the sense that
645 bacteria are set inactive until the root invades the soil node (Muci et al., 2012) or it is considered as a
646 boundary influx of soil bacteria (Dupuy & Silk, 2016). Contrastedly, models addressing the transport of
647 nutrients have had a stronger focus on the rhizosphere by using as input data 3D CT images of root
648 hairs in soil pores and they have demonstrated the benefits of such image-based modeling approaches
649 in understanding the uptake of phosphorus (e.g., Keyes et al., 2013; Roose et al., 2016). The

650 development of this type of model that includes the growth and metabolism of, e.g., beneficial bacteria,
651 pathogens or mycorrhiza is therefore urgently required to advance our understanding of the rhizosphere
652 and open up opportunities to control it to benefit crop production.

653

654 **5. Limitations of microscale models and future prospects**

655 We identified two major limitations that constitute severe challenges to microscale modeling efforts.
656 On one hand, available input data on soil architecture need to be sufficiently representative of reality
657 and to capture its essential features. On the other hand, the parameterization of biotic components of
658 these models needs to be sufficiently robust. In both respect, we shall identify research avenues that
659 could help fill current knowledge gaps and choose the most appropriate modeling strategies.

660

661 **5.1 Available input data on soil architecture**

662 The approaches that uses imaging of soil architecture are attractive because they preserve as much
663 as is practically feasible the real spatial arrangement of soil pores and provide realistic statistics on soil
664 physical properties. However, different image treatments (noise reduction, conversion into low number
665 of bits, segmentation algorithms) are applied to obtain binarized or ternary CT images on which most
666 of the image analyses are performed. These treatments can produce modifications of the bulk measures
667 of pore morphology such as porosity, specific surface area, or Euler connectivity (Houston et al., 2013).
668 Furthermore, small local changes of the size of key throats governing the water flux can dramatically
669 affect simulated hydrodynamic properties (Gackiewicz et al., 2019; Pot et al., 2020). Imaging data are
670 also limited by the pixel resolution attained by the different imaging tools, which can mask a
671 significant portion of soil porosity. At best, existing microscale models simulate microbial activity at a

672 scale of a few microns and while they can only capture a small part of the tremendous complexity of
673 soil architecture they miss out a lot of the sub-resolution pore space in which many bacteria, archaea,
674 and viruses reside. Baveye et al. (2017) report different strategies that can be used to consider the
675 unresolved pores from CT data and to describe their role in the carbon transformation. Among them is
676 the use of all the information contained in the gray-level pixels instead of using binarized images, or to
677 mix the traditional, binary approach with gray-scale modeling, as in the work of Yan et al. (2016,
678 2018). However, an implicit approach is necessary to assign a value for instance to the diffusion
679 coefficients in these pixels as a function of hydration or gas status. Multi-fractal approaches were
680 mentioned by Baveye et al. (2017) as a possible way to simulate the statistical distribution of
681 unresolved pores, but further analysis by Perrier et al. (2020) has recently demonstrated that their
682 potential was limited in this respect. Although we are still far from having handle on the sub-resolution
683 porosity, the approaches that have been explored so far at least confirm the importance of ‘hidden’
684 smaller pores in understanding soil processes and thereby encourage future research efforts. Recent
685 advances in imaging techniques should bring better knowledge of pore arrangement at the infra-micron
686 scale (Felde et al., 2020; Schlüter et al., 2019) and address their potential role in shaping soil microbial
687 activity.

688 An area of research that has recently emerged is the utilization of neural networks to predict
689 processes in rocks, using training data sets made of 3D binary CT images (Santos et al., 2020). To
690 improve training, geometrical features such as the Euclidean or transform distance map, the maximum
691 inscribed sphere flow, and tortuosity maps of the global paths along the flow direction are included in
692 the training data set. Rock architecture is far more homogeneous than is soil architecture, however the
693 convolutional neural network was able to deal to a reasonable extent with the higher heterogeneity

694 observed in rocks (dead-end pores, disconnected pores) compared to the initial training data set of bead
695 packs.

696 Another limitation comes from the fact that the spatial arrangement of soil constituents is highly
697 dynamic, continuously changing under the effect of biotic activity (including roots, macro-, meso-, and
698 micro-fauna) and abiotic stresses (e.g., drying-rewetting cycles). Time-resolved methods to image the
699 dynamics of soil architecture (e.g., Bottinelli et al., 2016) provide experimental data that can potentially
700 be used as direct model inputs. Recent attempts to simulate the evolution of soil architecture as a result
701 of microbial activity (Ray et al., 2017) or physico-chemical processes (Rupp et al., 2019), together with
702 research focusing on the role of roots in modifying the geometrical arrangement of soil particles
703 (Aravena et al., 2014; Kolb et al., 2017) will certainly open new avenues to bridge knowledge gaps.

704

705 **5.2 Parameterization of the biotic component**

706 A major concern that has not been discussed in any of the reviewed references deals with the
707 parametrization of the biological component. When models simulate the activity of a well-defined
708 microorganism, parameters describing its physiology are usually extracted from experimental data
709 measured in pure culture system. In doing so, models can only tackle a tiny part of the soil biodiversity.
710 Representative species of known functional groups are however modeled. A major difficulty in
711 extracting parameters from experiments is that the underlying mathematical formulations for the
712 growth kinetics used to describe the experimental growth curves are unevenly informative and
713 parameters extracted from these experimental studies can thus be in conflict with the formulation
714 adopted in a given microscale model (Vogel et al., 2018). We thus advocate to report them in
715 experimental studies. But even so, it is far from certain that the physiology of bacteria remains the

716 same whether the cells live freely or are attached to soil surfaces (e.g., Fletcher, 1979; Kirchman and
717 Mitchell, 1982; Lerch et al., 2017; Ulířová & Šantrůčková, 2003). Additionally, other parameters
718 associated to mortality and dormancy are generally obtained by calibration of macroscopic models
719 (e.g., Ingwersen et al., 2008) to experimental data from soil incubations with composite microbiota and
720 carbon sources (Vogel et al., 2018). These limitations render the use of these experimental data to
721 parameterize the biotic component very questionable.

722 The mobility of bacteria or fungi is also very difficult to parameterize. For bacteria, at best, data on
723 motility exist in artificial media (e.g., agar surfaces, micro-models), which may not be directly
724 transferable to motility in soil pores. Direct measurements in soils have demonstrated the impact of soil
725 architecture on the ability of bacteria to move (Juyal et al., 2018). These data, which describe the
726 movement of a population of bacteria, are directly transferable to models that do not adopt an explicit
727 description of soil architecture. For models accounting explicitly for soil architecture, this information
728 has to be used to calibrate/validate biotic parameters accounting for microbial movement, irrespective
729 of the formalism, either population- or individual-based.

730 In the case of fungi dispersal rates, hyphal expansion, and branching angles have been observed on
731 2D surfaces and incorporated into fungal models (Stacey et al., 2001). In theory these types of
732 parameterization can be expanded to 3D, however it has been shown that branching angles in a 3D pore
733 structure can significantly deviate from those reported in literature, suggesting that expansion of fungal
734 colonies has more complex feedback mechanisms with the environment than is currently considered in
735 models (Soufan et al., 2018).

736

737 **6 Conclusions**

738 Given the advantages and disadvantages of the different strategies used to describe soil micro-
739 environments, we recommend modeling benchmarks. Indeed, an explicit approach will not be able to
740 cope with the tremendous amount of data needed, and simplified approaches conserving the key spatial
741 arrangement of pores appears as a necessary alternative. Like Vogel et al. (2005) did in comparing a
742 pore-network model, a lattice-Boltzmann model and a morphological model to simulate the capillary
743 pressure of a soil sample whose topology was obtained by CT, and Pot et al. (2015) did in comparing a
744 lattice-Boltzmann model and a morphological model to simulate experimental spatial distribution of
745 air-water menisci as observed in synchrotron CT images, similar benchmark analyses should be carried
746 out with respect to soil microbial activity. Pure diffusion conditions (as those existing in standardized
747 soil incubation experiments) but also addition of intermittent water fluxes should be tested in modeling
748 scenarios. The latter should benefit from recent progress made in simplifying modelling of water flow
749 at pore scale for unsaturated conditions (Zhang et al., 2016).

750 In light of the complexity and uncertainty of soil processes as well as of imperfections of data
751 available, we also advocate for the use of a multimodal description of soil microhabitats along with a
752 modeling strategy involving data at different levels of description such as the so-called pattern-oriented
753 modeling (Grimm et al. 2005). The non-destructive imaging of soil properties and processes is rapidly
754 evolving and we need to find new ways of combining and including data emanating from these
755 techniques in the modeling process.

756 In this review we addressed the current practices used in soil science to account for soil architecture
757 and microbial dynamics at the scale of microbial habitats and address their advantages and
758 disadvantages. We will address in a forthcoming paper the insights gained by these models on soil
759 functions and discuss to what extent it is important to include the explicit description of soil
760 architecture in micromodels of soil microbial activity.

761

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766

767 **8 Data Sharing and Data Accessibility statement**

768 Data sharing is not applicable to this article as no new data were created or analyzed in this study.

769

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771

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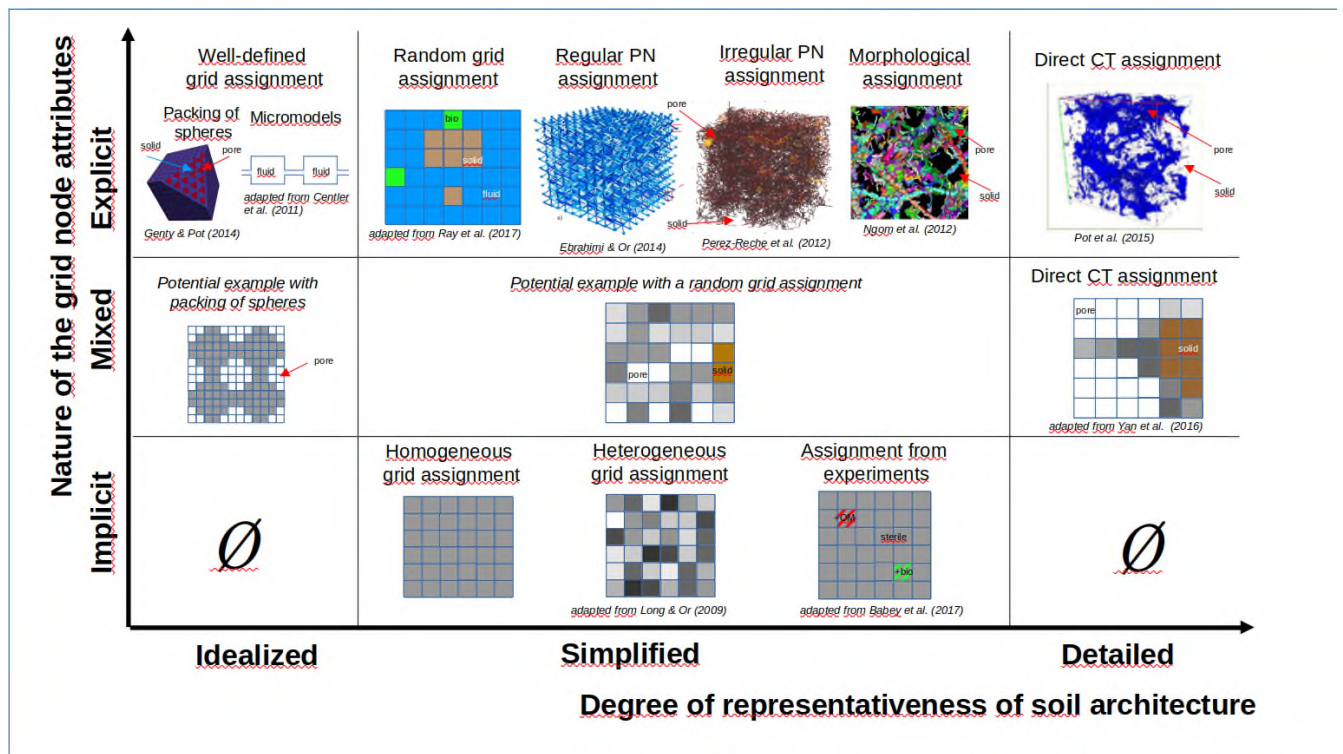
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1314 **Table 1:** Advantages and disadvantages of the different strategies used to describe soil micro-
1315 environments in pore-scale models of soil microbial dynamics. PN and OM are pore network and
1316 organic matter, respectively.

Modeling strategy for the description of soil microenvironments	Advantages	Disadvantages
Explicit node attributes / actual soil architecture	3D realistic soil architecture 3D realistic water-air distribution 3D realistic diffusion pathways 3D realistic location of OM and microorganisms Can deliver relationships between 3D soil architecture descriptors and soil microbial response	High volume of input data Computations intensive Small-scale simulation
Explicit node attributes / simplified soil architecture		
Case of morphological and irregular PN models	3D realistic diffusion pathways 3D realistic location of OM and microorganisms Larger-scale simulation Can deliver relationships between 3D soil architecture descriptors and soil microbial response	High volume of input data Approximate pore-solid interface Approximate air-water interface
Case of regular PN models	Low volume of input data (bulk soil parameters) Larger-scale simulation	Approximate 3D soil architecture Approximate 3D diffusion pathways
Case of regular grid	Low volume of input data (bulk soil parameters) Deliver simplified prototypes of models	Ignore actual 3D soil architecture Ignore actual 3D water-air distribution Ignore actual 3D diffusion pathways
Explicit node attributes / idealized soil architecture	Exact reproduction of experimental designs Model validation	Approximate actual 3D soil architecture
Mixed attributes / actual soil architecture	3D realistic soil architecture Take into account unresolved pores 3D realistic water-air distribution 3D realistic diffusion pathways 3D realistic location of OM and microorganisms	High volume of input data Computations intensive Small-scale simulation
Implicit node attributes / simplified soil architecture	Low volume of input data (bulk soil parameters) Larger-scale simulation Include space and dispersal in ecological interactions	Ignore actual 3D soil architecture Ignore actual 3D water and air distribution Ignore actual 3D diffusion pathways

Figure 1: Classification of pore-scale models of soil processes, according to the degree of representativeness of soil architecture (from idealized porous media to simplified architectures eventually to actual soils) and to the nature of the grid node attributes (implicit, explicit and mixed, i.e., both explicit and implicit). Implicit attributes are bulk porosity, water content and effective diffusion coefficients which values are represented by different levels of gray. Explicit attributes are local characteristics of the soil phases: solid, pores filled with air or pores filled with water, and molecular diffusion coefficients in air and water, which are represented by different colors. PN and CT are pore network and computed tomography, respectively. We added two potential examples of what would be a microscale model made of mixed attributes describing an idealized and a simplified soil architecture. The first one would be a packing of porous spheres described by explicit nodes (pore) and implicit nodes of constant local porosity and explicit nodes (the pore phase). The second one would be a random assignment of explicit nodes (pore and solid) and implicit nodes of varying local porosity that would fit the porosity of a soil sample. Microscale models using implicit attributes to describe either an idealized or a detailed soil architecture would be unrealistic cases and they are therefore indicated by the mathematical empty set symbol $\emptyset$.



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Accounting for soil architecture and microbial dynamics in microscale models: current practices in soil science and the path ahead

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