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# Modeling Population Patterns of Chemotactic Bacteria in Homogeneous Porous Media

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#### 6 Abstract

3

The spatio-temporal distribution of subsurface microorganisms determines their efficiency in providing essential ecosystem services such as the degradation of organic matter, the remineralization of carbon and nitrogen, or the 9 remediation of anthropogenic contaminants. Populations of motile, chemo-10 tactic bacteria have been shown to be capable of pattern formation even in 11 the absence of environmental heterogeneities. Focusing on the water satu-12 rated domain of the subsurface (e.q., aquatic sediments, porous aquifers), we 13 analyze this innate capability of bacterial populations in an idealized model 14 of a homogeneous, saturated porous medium. Considering a linear array of 15 connected, identical microhabitats populated by motile, chemotactic bacte-16 rial cells, we identify prerequisites for pattern formation, analyze types of 17 patterns, and assess their impact on substrate utilization. In our model, 18 substrate supplied to the microhabitats facilitates bacterial growth, and mi-19 crobial cells can migrate between neighboring microhabitats due to i) random 20 motility, ii) chemotaxis towards substrate, and iii) self-attraction. A precon-21 dition for inhomogeneous population patterns is analytically derived, stating 22 that patterns are possible if the self-attraction exceeds a threshold defined 23

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by the random motility and the steady state population density in the mi-24 crohabitats. An individual-based implementation of the model shows that 25 static and dynamic population patterns can unfold. Degradation efficiency 26 is highest for homogeneous bacterial distributions and decreases as pattern 27 formation commences. If during biostimulation efforts the carrying capac-28 ity of the microhabitats is successively increased, simulation results show that 29 degradation efficiency can unexpectedly decrease when the pattern formation 30 threshold is crossed. 31

32 Key words: pattern formation, ecosystem services, biodegradation,

<sup>33</sup> chemotaxis, individual-based modeling

#### 34 1. Introduction

Microbes inhabiting the subsurface domain drive many element cycles which 35 are essential for natural ecosystems and highly desirable from an anthropic 36 viewpoint. They are the main contributors to organic matter breakdown, 37 cycling of carbon and nitrogen, and degradation of organic contaminants 38 in the subsurface. The high spatial and temporal variability of the sub-30 surface domain poses a constant challenge to any microbial life present in 40 this habitat. As a consequence, the organization of subsurface microbial life 41 is complex. The spatial distribution of subsurface bacteria was shown to 42 be highly variable down to the micro-scale, suggesting that bacterial life is 43 inhomogeneously distributed, forming microbial 'hot spots' as local growth 44 conditions vary significantly (Bundt et al., 2001; Nunan et al., 2003). This 45 has profound implications for microbially mediated processes. Taking the 46 mircrobial degradation of contaminants as an example, only the fraction of 47

the contaminant can be degraded that comes into close physical contact with 48 the degrading bacteria. Accordingly, bacterial distribution affects contam-49 inant bioavailability and hence degradation efficiency (Harms and Bosma, 50 1997; Dechesne et al., 2010). In the saturated zone of the subsurface, where 51 the pore space is completely filled with water, as for example in aquatic 52 sediments and aquifers, degradation can be enhanced if bacteria are able 53 to detect contaminant concentration gradients and migrate towards regions 54 of higher concentrations. This process, called chemotaxis, has indeed been 55 shown to be beneficial in the context of bioremediation, where organic con-56 taminants serve as substrate for bacterial growth (Marx and Aitken, 2000; 57 Parales et al., 2000; Ford and Harvey, 2007; Wang et al., 2008). Bacteria 58 in soil often form microcolonies (Chenu et al., 2001; Dechesne et al., 2007). 59 These can originate from a single individual, or be dynamically formed by ac-60 tive aggregation. Such aggregation can be induced by bacterial self-attraction 61 mediated by the excretion of chemoattractants by the cells themselves (Mit-62 tal et al., 2003; Park et al., 2003). The amino acids aspartate and glycine 63 have been shown to act as such chemoattractants (Budrene and Berg, 1995; 64 Salman et al., 2006). High cell densities were shown to enhance resistance to 65 environmental stress, for example antibiotics (Butler et al., 2010), promote 66 gene transfer, and allow for efficient extracellular digestion. Furthermore, 67 bacterial aggregation facilitates quorum sensing induced coordinated behav-68 ior such as biofilm formation. The microenvironment engineered by bacterial 69 cells in aggregates provides a buffer against environmental fluctuations, en-70 hancing survival. Bacterial self-attraction has extensively been studied for its 71 pattern formation capacity in experiments (see e.g., Budrene and Berg, 1991,

1995; Ben-Jacob, 2003) and by mathematical modelling (see e.q., Keller and 73 Segel, 1970; Rosen, 1983; Woodward et al., 1995; Tyson et al., 1999; Painter 74 and Hillen, 2002). In these studies, however, usually only one chemotaxis pro-75 cess is considered, with Saragosti et al. (2010) presenting a recent exception 76 focusing on traveling pulses of bacteria. Even in homogeneous environments 77 where local growth conditions do not vary, bacterial distributions can be in-78 homogeneous and dynamic. In an experimental setup, Keymer et al. (2006) 79 studied a population of Escherichia coli cells colonizing a microfabricated lin-80 ear array of connected microhabitats. Rich metapopulation dynamics were 81 observed even if all microhabitats were equal in all parameters including sub-82 strate supply. The experimental setup resembles a saturated porous medium 83 as found in the natural subsurface, where microbial life is concentrated in 84 microhabitats which are connected to each other by micropores allowing for 85 diffusive substrate exchange and bacterial motion (Grundmann et al., 2001). 86 Inspired by these results, we consider a similar setup in this theoretical study. 87 Omiting and simplifying many aspects of natural saturated porous media as 88 microbial habitats including advection and spatial complexity, we define a ho-80 mogeneous environment in our model with identical microhabitats and evenly 90 distributed substrate supply. Under such conditions, any observed patterns 91 can be directly attributed to the system's innate pattern formation ability. 92 While following the experimental setup of Keymer et al. (2006) closely in the 93 formulation of our model, the aim of this work is not to reproduce experimen-94 tal results. Instead, we focus on first, identifying the determinants leading 95 to spatial distribution patterns in our model system as a substitute for a sat-96 urated porous medium, and second, on the impact on degradation efficiency 97

as a desired ecosystem service. While most modeling studies take only one chemotaxis process into account, we consider two competing chemotactic processes. Chemotaxis towards substrate leads to bacterial dispersal and enhanced degradation efficiency in a system with homogeneously distributed substrate supply, whereas self-attraction leads to bacterial aggregation. Note that survival advantages of bacterial aggregates will not be relfected in the model.

#### 105 **2. Model**

Following the experimental setup used by Keymer et al. (2006), we model a linear array of microhabitats resembling a saturated porous medium. A single bacterial species populates water filled microhabitats that are connected to the neighbouring microhabitats by channels, enabling bacterial cells to swim from one microhabitat to the next. Our model consists of two parts. The local model describes growth dynamics within microhabitats and the spatial model describes exchange processes between neighboring habitats (Figure 1).

Local Model. For modeling bacterial growth dynamics, we employ the model 113 already suggested by Keymer et al. (2006). Each microhabitat is treated as a 114 homogeneous, well-stirred reactor. Its current state at time t is characterized 115 by the number of bacterial cells occupying it  $p(t) \in [0, K]$  and substrate 116 concentration c(t). Assuming an upper limit  $c_{max}$  for substrate concentration, 117 substrate is considered in the model as a relative, unitless index s(t) :=118  $c(t)/c_{max} \in [0, 1]$ . Bacterial population dynamics is assumed to follow logistic 119 growth with the logistic term representing space limitation and an additional 120 dependency on substrate concentration (Keymer et al., 2006): 121

$$\frac{dp}{dt} = r(s) \cdot p \cdot \left(1 - \frac{p}{K}\right),\tag{1}$$

with carrying capacity K of a microhabitat and per capita growth rate r(s)for very small populations as defined by

$$r(s) = \mu s - d,\tag{2}$$

.

with parameter  $\mu$  describing bacterial growth under maximal substrate concentration (s = 1) and bacterial death controlled by parameter d. Substrate is supplied to the microhabitat by a generic capacitive process with rate parameter  $\lambda$  and consumed during bacterial growth in the microhabitat. Substrate dynamics is hence described by:

$$\frac{ds}{dt} = \lambda(1-s) - \varepsilon \mu s \frac{p}{K},\tag{3}$$

with bacterial conversion efficiency  $\varepsilon$ . Note that the population density p is expressed in cells per habitat. Hence, the consumption term must be scaled to the size of the microhabitat. Assuming that the carrying capacity K scales linearly with microhabitat size, we use it as a substitute for microhabitat size. This ensures that the same number of cells leads to the consumption of the same amount of substrate molecules, independent of microhabitat size. The full dynamics within one habitat is then described by:

$$\frac{dp}{dt} = (\mu s - d) \cdot p \cdot \left(1 - \frac{p}{K}\right) \qquad =: g(p, s) \tag{4}$$

$$\frac{ds}{dt} = \lambda(1-s) - \varepsilon \mu s \frac{p}{K} \qquad =: h(p,s). \tag{5}$$

Spatial Model. Bacterial migration between neighbouring microhabitats is 136 governed by three aspects. First, motile cells perform a random-walk move-137 ment as they swim through the fluid medium by rotating their flagella. This 138 process can be described as Fickian diffusion (Berg, 1983; Berg and Turner, 139 1990). The diffusive flux is  $J_D = -D_p \cdot \nabla p$ , with diffusion coefficient  $D_p$ . Sec-140 ond, cells respond to gradients in substrate concentration by directing their 141 movement towards locations of higher concentration. Usually, the chemo-142 tactic flux is described as  $J_C = \chi(c, p) \cdot \nabla c$ , with chemotaxis response func-143 tion  $\chi(c, p)$  and chemoattractant concentration c. For simplicity, we choose 144 a chemotaxis response function which is linear in population density and in-145 dependent from chemoattractant concentration. Choosing a constant sensi-146 tivity for chemotaxis to substrate  $\chi_s$ , our chemotactic flux towards substrate 147 becomes  $J_s = \chi_s \cdot p \cdot \nabla s$ . For the third aspect of cell motility, we assume that 148 bacterial cells excrete molecules that also act as chemoattractants. Instead 149 of considering the chemoattractant explicitly in the model, we assume that 150 its concentrations is proportional to bacterial cell density. Hence, the bac-151 terial flux due to self-attraction can be defined in analogy to the substrate 152 chemotaxis as:  $J_p = \chi_p \cdot p \cdot \nabla p$ , with sensitivity  $\chi_p$ . We assume a strictly 153 additive integration of both chemotactic processes (Saragosti et al., 2010). 154 The substrate is assumed to diffuse with diffusion coefficient  $D_s$ . Bringing 155 it all together, the spatial processes are described by two partial differential 156 equations: 157

$$\frac{\partial p}{\partial t} = D_p \cdot \nabla^2 p - \chi_s \cdot \nabla \cdot (p \nabla s) - \chi_p \cdot \nabla \cdot (p \nabla p) \tag{6}$$

$$\frac{\partial s}{\partial t} = D_s \cdot \nabla^2 s. \tag{7}$$

Note that the parameters  $D_p$ ,  $D_s$ ,  $\chi_p$ , and  $\chi_s$  are effective parameters that implicitely account for any flux restrictions imposed by the specific geometry of the corridors that connect neighboring microhabitats.

Full Model. Combining the spatial model (Equations 6 and 7) with the local
growth model (Equations 4 and 5) gives the full model:

$$\frac{\partial p}{\partial t} = D_p \cdot \nabla^2 p - \chi_s \cdot \nabla \cdot (p \nabla s) - \chi_p \cdot \nabla \cdot (p \nabla p) 
+ g(p, s) =: u(p, s) \quad (8) 
\frac{\partial s}{\partial t} = D_s \cdot \nabla^2 s 
+ h(p, s) =: v(p, s). \quad (9)$$

- <sup>163</sup> 3. Model Analysis
- 164 3.1. Local Model

The local model (Equations 4 and 5) has three steady states with  $g(p^*, s^*) = 0$ ,  $h(p^*, s^*) = 0$ :

$$(p_1^*, s_1^*) = (0, 1) \tag{10}$$

$$(p_2^*, s_2^*) = (K, \lambda/(\lambda + \varepsilon \mu))$$
(11)

$$(p_3^*, s_3^*) = (K\lambda/\varepsilon(1/d - 1/\mu), d/\mu).$$
(12)

The first steady state refers to the trivial case of bacterial extinction. In 167 the second steady state, the bacterial density is fixed to K, representing 168 carrying capacity limited growth. An increase in substrate supply  $\lambda$  does not 169 lead to an increase in population density, but only to an increase in substrate 170 concentration. In the third state however, an increase in substrate supply 171 translates into a larger population density, while substrate concentration is 172 fixed. This state refers to growth limited by substrate supply. To elucidate 173 the stability of these steady states, we perform a linear stability analysis. 174 The system is linearized around the steady state and the evolution of a small 175 perturbation is studied. If all eigenvalues of the system's Jacobian matrix are 176 negative, perturbations vanish with time. We find that asymptotic stability 177 is given under following conditions for the three steady states: 178

$$(p_1^*, s_1^*) : d > \mu \tag{13}$$

$$(p_2^*, s_2^*) : d < \mu \lambda / (\lambda + \varepsilon \mu) \tag{14}$$

$$(p_3^*, s_3^*): d < \mu, \varepsilon > \lambda(1/d - 1/\mu).$$
 (15)

The extinction case  $(p_1^*, s_1^*)$  is only asymptotically stable if the parameter 179 controlling death d exceeds the parameter controlling growth  $\mu$ . The opposite 180 must be true for the other two steady states to become stable. For the second 181 steady state  $(p_2^*, s_2^*)$ , parameter d is even more limited, as  $\lambda/(\lambda + \varepsilon \mu) < 1$ . 182 This inequality can be rewritten as  $d < \mu s_2^*$ . For the substrate limited steady 183 state  $(p_3^*, s_3^*)$ , the substrate conversion efficiency must exceed a threshold 184 defined by the parameters for substrate supply, bacterial growth and death. 185 This inequality can be rewritten to  $p_3^* < K$ . While the eigenvalues for the 186

first two steady states are never complex, the eigenvalues for the third steady 187 state can be complex for certain parameter settings<sup>1</sup>, indicating oscillatory 188 behavior. For a specific example, parameter regions with signs of eigenvalues 189 are shown in Figure 2 for steady states two and three. The bifurcation 190 diagram in Figure 3 illustrates how the system undergoes a transcritical 191 bifurcation. For large values of  $\lambda$ , steady state two is asymptotically stable 192 and steady state three unstable. Decreasing  $\lambda$ , the stability properties are 193 switched at the bifurcation point, where saddle nodes collide with stable 194 nodes. Decreasing  $\lambda$  further, a second bifurcation occurs for steady state 195 three where the stable node becomes a stable spiral. 196

#### 197 3.2. Full Model

Mass exchange between microhabitats in the full model is driven by spatial 198 gradients. If all microhabitats have identical population densities and sub-199 strate concentrations, spatial gradients vanish and exchange processes will 200 not change the system's state. Hence, if the spatial model is homogeneously 201 initialized with population densities and substrate concentrations of a steady 202 state of the local model, also the full model is at steady state. To assess the 203 stability of the steady state in the full model, a second linear stability analy-204 sis needs to be performed. Again, we have to analyze whether a perturbation 205 of the spatial system in steady state is amplified or decays over time. In cases 206 where perturbations do not fade, spatial patterns can emerge. We restrict 207 our analysis to a one-dimensional domain of length L with spatial coordi-208 nate x. We follow the evolution of small perturbations around any spatially 209

 $^{-1}\lambda < 4d^{2}(\mu - d)/\mu^{2}, \ \varepsilon > 4\lambda d(\mu - d)^{2}/(\mu(4d^{2}(\mu - d) - \lambda\mu^{2}))$ 

homogeneous steady state  $(p(x), s(x)) = (p^*, s^*)$ , which is assumed to be asymptotically stable in the local model. We define the perturbation as:

$$d(x,t) := \begin{pmatrix} p(x,t) - p^* \\ s(x,t) - s^* \end{pmatrix}.$$
 (16)

<sup>212</sup> The time evolution of the perturbation d is given by

$$\frac{\partial d}{\partial t} = Ad$$

$$= \begin{pmatrix} u_p & u_s \\ v_p & v_s \end{pmatrix}_{p^*, s^*} d$$

$$= \begin{pmatrix} D_p \nabla^2 - \chi_p p^* \nabla^2 + g_p^* & -\chi_s p^* \nabla^2 + g_s^* \\ h_p^* & D_s \nabla^2 + h_s^* \end{pmatrix} d, \quad (17)$$

with  $u_p$  denoting the partial derivative of u with respect to p, and  $u_s, v_p, v_s$ accordingly, and writing  $g_p^*$  short for  $g_p(p^*, s^*)$ , and  $g_s^*, h_p^*, h_s^*$  accordingly. With solutions of the form  $d \sim \cos(kx)e^{\lambda t}$ , with wavenumber  $k = n\pi/L$ , n a whole number, the sign of  $\lambda$  decides on the fate of the perturbation. From the solution follows:  $\nabla^2 d = -k^2 d$ . Setting this into Equation 17, we can compute  $\lambda$  as the eigenvalues of A. They are determined by:

$$\begin{vmatrix} -k^2 D_p + k^2 \chi_p p^* + g_p^* - \lambda & k^2 \chi_s p^* + g_s^* \\ h_p^* & -k^2 D_s + h_s^* - \lambda \end{vmatrix} = 0.$$
(18)

<sup>219</sup> This leads to:

$$\lambda^2 + a(k^2)\lambda + b(k^2) = 0, \text{ with}$$
(19)

$$a(k^{2}) = (D_{s} + D_{p} - \chi_{p}p^{*})k^{2} - (g_{p}^{*} + h_{s}^{*})$$

$$b(k^{2}) = (D_{p} - \chi_{p}p^{*})D_{s}k^{4} - (D_{p}h_{s}^{*} + \chi_{s}p^{*}h_{p}^{*} - \chi_{p}p^{*}h_{s}^{*} + D_{s}g_{p}^{*})k^{2} +$$

$$g_{p}^{*}h_{s}^{*} - g_{s}^{*}h_{p}^{*}.$$
(20)
(21)

Spatial patterns can form if  $\lambda$  has positive real components, as perturbations 220 do not fade in this case. This is true if  $a(k^2) < 0$  or  $b(k^2) < 0$ . Assuming 221 that the steady state  $(p^*, s^*)$  is asymptotically stable in the local model, it 222 follows that both of its eigenvalues  $\lambda_l^{1,2}$  are negative in the local model. From 223  $\begin{vmatrix} g_p^* - \lambda_l & g_s^* \\ h_p^* & h_s^* - \lambda_l \end{vmatrix} = 0, \text{ with } \lambda_l^{1,2} < 0 \text{ follows: } g_p^* + h_s^* < 0, g_p^* h_s^* - g_s^* h_p^* > 0.$ 224 Using this we find that  $a(k^2) < 0$  for  $k > k_{crit}$ , if  $D_s + D_p - \chi_p p^* \leq 0$ . 225 Furthermore,  $b(k^2) < 0$  is guaranteed for  $k > k'_{crit}$ , if  $D_p - \chi_p p^* < 0$ . And 226 finally for  $D_p - \chi_p p^* > 0$ ,  $b(k^2)$  might still become negative for  $k_{crit,l} < k < 0$ 227  $k_{crit,h}$ . Concluding, spatial patterns are in principle possible for  $D_p - \chi_p p^* > 0$ 228 0, albeit under a limited choice of wave numbers k. This limitation is relaxed 229 for 230

$$D_p - \chi_p p^* < 0. (22)$$

<sup>231</sup> Under this condition, spatial patterns can be expected.

#### 232 4. Individual-Based Model Implementation

Microcolonies consisting of very few individual cells have been reported in the subsurface (Chenu et al., 2001; Grundmann, 2004). Since differential equation based modeling is not applicable to populations of few cells and

additionally, blow up is a problem in chemotaxis modeling using partial dif-236 ferential equations (see e.q., Perthame, 2007), we follow an individual-based 237 approach. This approach has been successfully applied in microbial ecology, 238 for example in the context of biofilms (see e.q., Kreft et al., 2001; Mabrouk 239 et al., 2010). The differential equation based full model focusing on the 240 population level is converted into a stochastic model implementation focus-241 ing on the single cell level for computational simulations. The simulation 242 loop consists of two steps: First, the growth dynamics is simulated for each 243 microhabitat in the array. In the second step, bacterial migration between 244 neighboring microhabitats, and substrate diffusion is simulated. Within the 245 individual-based simulation, each bacterial cell is considered separately. Bac-246 terial processes considered in the model are not assumed to depend on a 247 specific state of the cells such as age or size, so that cells can be modeled as 248 stateless entities. For the local model, we need to derive probabilities for the 249 stochastically independent events of cell division  $P_{\mu}$  and cell death  $P_d$  during 250 each step of the simulation of length  $\Delta t$ . Rewriting Equation 4 as 251

$$\frac{dp}{dt} = p \cdot \left(\mu s - (\mu s - d)\frac{p}{K}\right) - p \cdot d \tag{23}$$

<sup>252</sup> allows us to assign the probabilities as:

$$P_{\mu} := \left(\mu s - (\mu s - d)\frac{p}{K}\right) \cdot \Delta t \tag{24}$$

$$P_d := d \cdot \Delta t. \tag{25}$$

In the first step of the simulation loop, each bacterial cell has the chance
to divide and die, in accordance with these probabilities. For each bacterial

cell, two uniformly distributed random numbers  $r_{\mu}$  and  $r_d$  are drawn over the intervall [0, 1]. The cell divides in case of  $r_{\mu} < P_{\mu}$  and (additionally) dies in case of  $r_d < P_d$ . The time step size has to be small enough to ensure  $P_{\mu}$ and  $P_d \ll 1$ . To derive probabilities for the migration of bacteria, we apply the standard central difference scheme to Equation 6. The resulting equation can be arranged to:

$$p_i^{t+\Delta t} = P_0 \cdot p_i^t + P_1 \cdot p_{i+1}^t + P_2 \cdot p_{i-1}^t, \tag{26}$$

261 with

$$P_{0} = 1 - \frac{2D_{p}\Delta t}{(\Delta x)^{2}} - \frac{\chi_{s}\Delta t}{(\Delta x)^{2}}(s_{i+1} - 2s_{i} + s_{i-1}) - \frac{\chi_{p}\Delta t}{(\Delta x)^{2}}(p_{i+1} - 2p_{i} + p_{i-1})$$
(27)

$$P_1 = \frac{D_p \Delta t}{(\Delta x)^2} - \frac{\chi_s \Delta t}{4(\Delta x)^2} (s_{i+1} - s_{i-1}) - \frac{\chi_p \Delta t}{4(\Delta x)^2} (p_{i+1} - p_{i-1})$$
(28)

$$P_2 = \frac{D_p \Delta t}{(\Delta x)^2} - \frac{\chi_s \Delta t}{4(\Delta x)^2} (s_{i-1} - s_{i+1}) - \frac{\chi_p \Delta t}{4(\Delta x)^2} (p_{i-1} - p_{i+1}), \quad (29)$$

where  $p_i^t$  describes the number of bacterial cells in microhabitat *i* at time *t*, 262  $s_i$  describes the substrate concentration in habitat i at time t and  $\Delta x$  de-263 scribes the distance between neighboring microhabitats. We follow Schofield 264 et al. (2002) who take the coefficients  $P_0, P_1$ , and  $P_2$  to be proportional to 265 the probability for a bacterial cell to remain at its current microhabitat  $(P_0)$ , 266 move to the left microhabitat  $(P_1)$ , and move to the right microhabitat  $(P_2)$ . 267 For simulating cell migration in each time step, a random number q is drawn 268 for each bacterial cell in the array that is uniformly distributed over the in-269 terval  $[0, \sum_k P_k]$ . For  $q \in [0, P_0]$ , the cell remains in its current microhabitat, 270

for  $q \in [P_0, P_1]$ , the cell migrates to the left neighboring microhabitat and for 271  $q \in [P_1, P_2]$  it migrates to its right neighbor microhabitat. In order to avoid 272 boundary effects at the edge of the microhabitat array, we employ periodic 273 boundary conditions in which the array is wrapped around forming a ring, so 274 that the rightmost habitat has the leftmost habitat as its right neighbor. If, 275 after all migratory events have been performed, a habitat contains more cells 276 than its carrying capacity K, cells are randomly moved from the overcrowded 277 habitat to its neighboring habitats until all habitats contain at most K cells. 278 For the substrate diffusion, the standard central difference scheme is directly 279 applied to Equation 7. 280

Parameter Settings. We simulate an array of 80 microhabitats. All pa-281 rameter values are summarized in Table 1. The parameters for the local 282 model are taken from Keymer et al. (2006) who fitted them to experimen-283 tal data for a single habitat. With these parameter settings, only the third 284 steady state, referring to substrate limited growth, is asymptotically stable 285 with  $(p_3^*, s_3^*) = (2747 \text{ cells}, 0.394)$ . This steady state is a stable spiral. For 286 the diffusion coefficient for substrate, we choose a value which is typical for 287 small molecules (Berg, 1983), for example toluene or benzene. For the dif-288 fusion coefficient of the bacteria and their chemotactic sensitivity towards 289 the substrate, we use experimentally derived values from Berg and Turner 290 (1990). They set up capillary tubes with a diameter of 10  $\mu$ m to simulate 291 a porous medium consisting of straight pores. We vary the sensitivity for 292 self-attraction over one order of magnitude. For the upper limit, we assume 293 that the self-attraction migration flux does not exceed the flux due to chemo-294 taxis towards substrate, as the response to substrate is supposed to be the 295

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most pronounced due to its direct evolutionary advantage. Assuming the 296 maximum gradients for bacterial cells and substrate concentration, the con-297 tributions of both chemotactic processes to the migration probability become 298 equal if setting  $\chi_p^{max} = \chi_s/K$ . This defines the upper limit of the chemo-299 tactic sensitivity for self-attraction. In all simulation runs of the full model, 300 each microhabitat in the array is initialized at steady state three of the local 301 model with  $((p^{t_0}, s^{t_0}) = (2747, 0.394)).$ 302 CÍ

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#### 5. Simulation Results 303

#### 5.1. Bacterial Growth in the Local Model 304

First, only growth within a single habitat is considered and the deterministic 305 solution of the local model (Equations 4 and 5) is compared to ten indepen-306 dent runs of the individual-based model. The system is initialized either with 307 ten bacterial cells and maximal substrate concentration  $((p^{t_0}, s^{t_0}) = (10, 1.0))$ 308 or at steady state three  $((p^{t_0}, s^{t_0}) = (2747, 0.394))$ . In the former case (Fig-309 ure 4, left), a damped oscillation around the steady state is visible after a 310 first exponential growth phase, in accordance with steady state three be-311 ing a stable spiral. The stochastic runs generally follow the deterministic 312 dynamics with stochastic fluctuations leading to a time offset and varying 313 amplitudes, scattered around the deterministic amplitude. An erratic oscil-314 lation of the stochastic system around the deterministic solution is visible 315 when the system is initialized at steady state three (Figure 4, right). 316

#### 317 5.2. Homogeneous Bacterial Distributions in the Full Model

According to Equation 22, homogeneous bacterial distributions can be ex-318 pected for the chosen parameter set if the chemotactic sensitivity towards 319 the chemoattractant  $\chi_p$  is below the critical value of  $\chi_p^* = 1.89 \times 10^{-9} \text{cm}^2/\text{s}$ . 320 In this case, the whole microhabitat array is homogeneously populated over 321 time except for stochastic fluctuations (Figure 5, left). If considering the 322 evolution of mean values over all microhabitats, an oscillation in population 323 density and substrate concentration close to the local steady state three be-324 comes apparent (Figure 5, right). A high population density is followed by a 325 decrease in substrate concentration, which in turn leads to a decreasing pop-326 ulation. This allows the microhabitat to recover. With the ensuing increase 327 in population density, the circle is closed. In this case, the mean dynamics 328 of the whole system resembles the local dynamics. The array can be thought 329 of as operating as one large microhabitat. 330

#### 331 5.3. Pattern Formation

If the chemotactic sensitivity  $\chi_p$  is set to values above the pattern formation 332 threshold  $\chi_p^*$ , inhomogeneous spatial population distributions emerge. In the 333 transition from homogeneous distributions to spatial structures, four types 334 of distinct spatio-temporal distribution patterns can be distinguished (Fig-335 ure 6). Pattern formation starts shortly before the threshold  $\chi_p^*$  is reached. 336 In the first pattern type, few microhabitats spontaneously become saturated 337 with bacterial cells. Microhabitats in the vicinity of these static hot spots 338 are depleted in bacteria, while distant microhabitats are still homogeneously 339 populated. As  $\chi_p$  is increased, more and more static hot spots form, until 340 hot spots start to repeatedly form and disintegrate in Pattern Type 2. The 341

remaining microhabitats synchronously oscillate in population density. The 342 formation of new hot spots is triggered by peaks in mean population density, 343 whereas disintegration is induced by low mean densities. While some hot 344 spots last for only one oscillation, others prevail over longer time periods. 345 As  $\chi_p$  is further increased, only few evenly distributed hot spots form in 346 the array in Pattern Type 3 of the transition. They span up to two micro-347 habitats and occasionally shift to neighboring microhabitats. Increasing  $\chi_p$ 348 further leads to a dense pattern of static hot spots next to almost completely 349 vacated microhabitats in the final Pattern Type 4 of the transition. The 350 four transition pattern types also show distinct dynamics in the mean be-351 havior of the whole array (Figure 7). The trajectory of the mean population 352 density and mean substrate concentration in Pattern Type 1 remains in the 353 vicinity of the local steady state three, albeit shifted to a state of slightly 354 lower density and higher substrate concentration. The dynamic pattern of 355 Pattern Type 2 corresponds to a pronounced oscillation of the mean trajec-356 tory. As few moving hot spots form in Pattern Type 3, the mean trajectory 357 settles in an oscillation of small amplitude far away from steady state three 358 after an initial transient phase. For Pattern Type 4, the mean trajectory 359 settles in an oscillation around a state of lower density and higher substrate 360 concentration compared to steady state three, albeit in closer proximity to 361 it than in Pattern Type 3. Here, the amplitude of the oscillation is smaller 362 compared to the oscillation in the spatially homogeneous case (cf. insets in 363 Figure 7 and Figure 5, right). Mean population density per microhabitat 364 steadily decreases during the first three pattern types of the transition. Al-365 though density begins to recover in the Pattern Type 4, the level achieved 366

under homogeneous colonization is not reached again (Figure 8). Due to fast 367 substrate diffusion, substrate gradients remain small in the microhabitat ar-368 ray and play a minor role in bacterial migration. A decrease by a factor of 50 369 brings the substrate diffusion coefficient into the range that has been reported 370 for the herbicide atrazine in soil (Ritter et al., 1973). Under these conditions, 371 substrate gradients affect bacterial migration. A typical simulation run with 372  $\chi_p > \chi_p^*$  is shown in Figure 9. At the beginnig of the simulation, a tran-373 sient checkerboard pattern unfolds. Substrate is faster consumed in highly 374 populated microhabitats. This makes neighboring microhabitats of lower cell 375 densities more and more attractive, eventually leading to a migration to these 376 microhabitats. Vacated microhabitats recover in substrate concentration due 377 to permanent substrate supply, again becoming attractive for recolonization. 378 After approximately ten minutes, traveling waves emerge that sweep through 379 the array, attracted by fresh microhabitats and leaving substrate depleted mi-380 crohabitats behind. On collision, migratory waves create temporal hot spots 381 that finally dissolve and release further migration waves. Despite the highly 382 structured spatio-temporal bacterial distribution, the mean behavior of the 383 whole array shows little variability (Figure 9, right). As bacterial activity is 384 concentrated in few microhabitats, an overall state of lower mean population 385 density and higher mean substrate concentration is assumed in comparison 386 to the local steady state three. 387

#### 388 5.4. Effect of Biostimulation on Substrate Utilization

In order to enhance the remediation of contaminated field sites, biostimulation has been proposed (Wenderoth et al., 2003). For example, additional terminal electron acceptors can be injected into the contaminated subsurface

to stimulate growth of degrading bacteria. In our model, the carrying capac-392 ity K describes the maximum number of cells that can be supported in one 393 microhabitat. This limit depends on microhabitat size, and can additionally 394 also depend on further requirements for bacterial growth, for example ter-395 minal electron acceptors such as nitrate or sulfate, which are not explicitly 396 considered in our model. Hence, an addition of terminal electron accep-397 tors translates into an increase of K in our model. Combining the pattern 398 formation condition Equation 22 with the condition for steady state three 399 representing substrate limited growth (Equation 12) leads to: 400

$$D_p < K\chi_p \lambda/\varepsilon \cdot (1/d - 1/\mu) \tag{30}$$

as the condition for pattern formation. This formulation makes it evident 401 that an increasing value of K due to biostimulation efforts can lead to the 402 pattern formation condition to become true and hence the emergence of spa-403 tially inhomogeneous bacterial population patterns. To evaluate the resulting 404 effect on substrate degradation as an desired ecosystem function, we perform 405 a series of simulation runs with increasing K values and consider the mean 406 consumption rate and mean population density over the whole array and en-407 tire simulation time, excluding the initial transient phase (Figure 10). The 408 consumption rate is computed as substrate concentration decrease due to mi-409 crobial growth (second summand in Equation 5, but without scaling factor 410 K). Chemotactic sensitivity towards chemoattractant is set to  $1.3 \times 10^{-9}$ 411  $cm^2/s$ . Under these parameter settings, the pattern formation threshold for 412 the carrying capacity K is  $K^* = 14560$  bacterial cells. The response to bios-413 timulation can be divided into three stages (Figure 10). For low K values, 414

the array is homogeneously populated and its dynamics follows the dynamics 415 of the local model. An increase in K leads to a linear increase in popula-416 tion density and consumption rate. As the pattern formation threshold  $K^*$ 417 is almost reached, the population density and consumption rate decrease, 418 despite the availability of better growth conditions due to larger K values. 419 As bacterial activity becomes concentrated in hot spot microhabitats, sub-420 strate available in microhabitats of low bacterial density is no longer utilized. 421 Hence, the onset of spatial pattern formation leads to a nonlinear response to 422 biostimulation. The trend is reversed at K values above 16000 cells, where 423 the linear response resumes. As more and more fully saturated microhabitats 424 form, more substrate can be utilized. However, the maximum consumption 425 rate given by steady state three of the local model cannot be reached again 426 once the pattern formation threshold has been crossed. 427

#### 428 6. Discussion

Studying the dynamics of a single bacterial species colonizing a linear ar-420 ray of connected microhabitats in a simplistic model resembling a saturated 430 porous medium led to three main results. The first result was obtained by 431 an analytical analysis that revealed a critical threshold above which spatially 432 inhomogeneous population patterns are possible. The existence of patterns 433 depends on the relation between bacterial parameters and environmental fac-434 tors. This becomes apparent if the pattern formation condition (Equation 30) 435 is rewritten as: 436

$$\underbrace{\varepsilon \frac{\mu d}{\mu - d}}_{\text{bacterial physiology}} \cdot \underbrace{\frac{D_p}{\chi_p}}_{\text{environmental factors}} < \underbrace{K \cdot \lambda}_{\text{environmental factors}}.$$
(31)

This relation indicates that for fixed environmental factors, faster bacterial 437 growth, a lower random motility, as well as an increased affinity to fellow 438 bacteria will increase the likelihood of inhomogeneous bacterial distributions. 439 The parameter values for bacterial growth and death used in the simulations 440 were taken from experimental data on E. coli cells. The chosen maximal 441 bacterial growth rate of  $0.15 \text{ min}^{-1}$  is beyond the capacity of typical soil 442 bacteria. If both growth and death rate are reduced by the same factor to 443 values more realistic for soil bacteria, the growth term in Equation 31 gets 444 reduced by the same factor. This shifts the pattern formation threshold 445 to lower values of  $\chi_p$ , making inhomogeneous distributions more probable. 446 This trend however is counteracted if for the environmental factors a lower 447 carrying capacity or substrate supply rate is chosen, in accordance with sub-448 strate usually being scarce in subsurface environments. Bacterial physiology 449 parameters can vary between bacterial species. Hence, under a given envi-450 ronment, one species might tend to form patterns while the other does not. 451 And vice versa, if environmental factors vary over space and time, a species 452 might tend to form patterns only in specific locations and during distinct 453 periods of time. Both the diffusion constant for substrate and the chemotac-454 tic sensitivity towards the substrate do not appear in the pattern formation 455 condition. Under the homogeneous environment conditions considered in 456 our model, they hence have no influence on the existence of patterns in the 457

model. As the second result of this study, the potential types of spatio-458 temporal patterns were identified using individual-based simulation runs. It 459 is well known that complex patterns can spontaneously emerge in coupled 460 reaction-diffusion systems even under homogeneous environments (Turing, 461 1952). Turing patterns of bacteria have already been reported in a sediment 462 modeling study by Baurmann et al. (2004). For parameter settings far away 463 from the pattern formation threshold, static patterns emerged in our model: 464 homogeneous bacterial distributions if parameters were set to values below 465 the threshold, and a pattern of saturated microhabitats next to virtually 466 empty microhabitats if parameter values exceeded the threshold. The whole 467 array operates as one large microhabitat for homogeneous bacterial distri-468 butions. For inhomogeneous distributions, the mean behavior of the whole 469 microhabitat array deviates from the local model's dynamics and a state 470 of lower mean population density and higher mean substrate concentration 471 is assumed. Furthermore, the variability of mean bacterial population and 472 substrate concentration over time was reduced in these cases. Hence, un-473 der pattern formation, the spatial interactions exerted a stabilizing effect on 474 habitat dynamics. Dynamic patterns were found for parameter values in the 475 vicinity of the pattern formation threshold. In particular, if substrate diffu-476 sion was decreased, dynamic checkerboard and wave patterns emerged. Such 477 wave like motions have also been observed in experimental setups (Keymer 478 et al., 2006; Saragosti et al., 2010). As the third result of this study, the onset 479 of pattern formation was found to cause a non-linear response to biostimu-480 lation efforts. It has been experimentally shown that aggregated bacterial 481 distribution patterns lead to reduced biodegradation (Dechesne et al., 2010). 482

A similar phenomenon was observed in our model. Biodegradation efficiency 483 decreased as the pattern formation threshold was exceeded and the bacterial 484 distribution became inhomogeneous. As bacterial activity becomes concen-485 trated in few hot spots, substrate in microhabitats of low bacterial density 486 is no longer degraded efficiently. This fraction of the substrate is no longer 487 bioavailable due to the absence of bacteria, and the overall degradation per-488 formance falls short of the expectation derived from the local dynamics. This 489 is a common observation when applying laboratory results to the field-scale. 490 In our model, pattern formation is the cause leading to reduced bioavailability 491 and hence, reduced overall degradation performance. In a field application, 492 however, the non-linear response to biostimulation can only be observed if the 493 microhabitats are homogeneously colonized in the pristine state. And even 494 then, it could be argued that by further increasing biostimulation after the 495 onset of pattern formation and an ompanying decrease in degradation per-496 formance, the linear response will resume. In this study, a simplistic model 497 has been used that omits and simplifies many aspects of the subsurface as 498 a bacterial habitat. For example, a water phase was assumed to be present 490 that connects neighbouring microhabitats, advection has been neglected, and 500 microhabitats were identical, mimicking a homogeneous environment. Fur-501 thermore, microhabitats were treated as well-mixed, neglecting any sub-scale 502 spatial features, and only a single bacterial species has been considered in 503 contrast to the tremendous diversity of soil bacteria. These simplifications, 504 however, allowed us to analytically derive a condition for pattern formation, 505 and uncover mechanisms driving spatio-temporal bacterial distribution, that 506 are also plausible driving forces for the dynamics in real soil systems. Bacte-507

rial growth was modeled following a modified logistic growth model suggested 508 by Keymer et al. (2006). Note however, that the analytical derivation of the 509 pattern formation condition did not depend on a particular growth model. 510 The existence of an asymptotically stable steady state was the only assump-511 tion regarding the local growth model. Hence, the results are also valid 512 if a different growth model is used, for example if bacterial growth follows 513 Monod-type kinetics. The model can easily be extended to become a more 514 faithful representation of the subsurface environment. Spatial inhomogeneity 515 of the environment can be included by varying carrying capacity and sub-516 strate inflow over microhabitats. The influence of heterogeneities imposed by 517 the environment on the innate pattern formation capability of bacterial pop-518 ulations can then be studied. Furthermore, an additional bacterial species 519 can be included. In such a scenario, bacterial interactions and coexistence in 520 spatially structured environments can be assessed. If parameters describing 521 bacterial physiology including chemotactic sensitivities are subjected to ran-522 dom mutations on cell division, the evolution of survival strategies of both 523 species can be analyzed. In the presented work, mathematical and computa-524 tional modeling was applied as a suitable tool to advance our understanding 525 of the dynamics of microbial processes in the subsurface. While not all pa-526 rameters of interest are necessarily available at the desired spatio-temporal 527 resolution in experimental setups, computational models are not constrained 528 by such limitations. This makes them well suited to identify key mechanisms 529 behind microbially driven dynamics in the subsurface. 530

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#### 635 Tables

Table 1: Parameter values for individual-based simulations, based on typical values for

E.	coli

Parameter		Value		Reference		
$\mu$	bacterial growth	0.15	$\min^{-1}$	Keymer et al. (2006)		
d	bacterial death	0.059	$\min^{-1}$	Keymer et al. (2006)		
K	carrying capacity of microhabitats	10000	cells	Keymer et al. (2006)		
$\lambda$	substrate inflow	0.004	$\min^{-1}$	Keymer et al. (2006)		
ε	conversion efficiency	0.15		Keymer et al. $(2006)$		
$D_s$	substrate diffusion coefficient	$9  imes 10^{-6}$	$\mathrm{cm}^2/\mathrm{s}$	Berg (1983)		
$D_p$	bacterial diffusion coefficient	$5.19\times10^{-6}$	$\mathrm{cm}^2/\mathrm{s}$	Berg and Turner (1990)		
$\chi_s$	chemotactic sensitivity to substrate	$1.3  imes 10^{-3}$	$\mathrm{cm}^2/\mathrm{s}$	Berg and Turner $(1990)$		
$\chi_p$	chemotactic sensitivity to bacteria	$1.3 \times 10^{-9}$ –	$1.3 \times 10^{-1}$	$0^{-8} \text{ cm}^2/\text{s}$		
$\Delta x$	distance between microhabitats	0.005	cm	Keymer et al. $(2006)$		
$\Delta t$	time step size	1	$\mathbf{S}$			
Recept						

#### 636 Figures



Figure 1: Key processes considered in the local (left) and spatial part (right) of the full model. Substrate supply to microhabitats is controlled by the rate parameter  $\lambda$ , bacterial cells consume substrate with conversion efficiency  $\epsilon$  and undergo cell divisions and cell death controlled by the rate parameters  $\mu$  and d, respectively. Microhabitats are treated as well-stirred reactors that can hold a maximum of K cells. In a linear arrangement, neighboring habitats are connected by corridors through which substrate diffuses and cells can migrate due three processes, controlled by parameters as indicated.



Figure 2: Stability of steady states two and three of the local model using values for parameters  $\mu$ , d, and K as given in Table 1. The signs of the two eigenvalues are shown for steady state two (left) and steady state three (right) in  $\lambda - \varepsilon$  parameter space. Regions with saddle nodes are marked with (-,+), regions with stable nodes with (-,-), and regions with stable spirals with (-,-)\*.



Figure 3: Bifurcation diagram for the local model using parameter values given in Table 1. Stable node as solid line, saddle point as dotted line, and stable spiral as dash-dotted line. For large  $\lambda$  values, steady state two  $(p_2^*, s_2^*)$  is asymptotically stable, and steady state three  $(p_3^*, s_2^*)$  is unstable. When decreasing  $\lambda$ , stability properties are first swapped at a transcritical bifurcation, and a further bifurcation ends in a stable spiral for steady state three.



Figure 4: Growth dynamics in the local model. The deterministic solution of the local growth model is compared to ten independent individual-based model runs. The system is initialized either with ten bacterial cells and maximal substrate concentration (left), or at steady state three  $(p_3^* = 2747, s_3^* = 0.394)$  (right).

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Figure 5: Homogeneous bacterial distribution for simulation runs with  $\chi_p < \chi_p^*$ . Spatio-temporal bacterial distribution (left), and mean behavior of the whole array over time (right) for a typical simulation run with  $\chi_p = 1.3 \times 10^{-9} \text{ cm}^2/\text{s}$ . The mean values oscillate around steady state three of the local model (right, inset). The system is homogeneously initialized in steady state three, and all other parameters are given in Table 1.



Figure 6: Spatio-temporal bacterial distribution patterns for individual simulation runs representing the four types of pattern as the pattern formation threshold  $\chi_p^*$  is exceeded. Pattern formation commences shortly before  $\chi_p^* = 1.89 \times 10^{-9} \text{ cm}^2/\text{s}$  is reached and leads to few static hot spots in Pattern Type 1 ( $\chi_p = 1.71 \times 10^{-9} \text{ cm}^2/\text{s}$ ), transient hot spots in Pattern Type 2 ( $\chi_p = 1.91 \times 10^{-9} \text{ cm}^2/\text{s}$ ), moving hot spots in Pattern Type 3 ( $\chi_p = 2.07 \times 10^{-9} \text{ cm}^2/\text{s}$ ), and dense static hot spots in Pattern Type 4 ( $\chi_p = 1.3 \times 10^{-8} \text{ cm}^2/\text{s}$ ). The system is homogeneously initialized in steady state three, and all other parameters are given in Table 1.



Figure 7: Temporal evolution of mean behavior over space of bacterial population and substrate concentration. Shown data are individual simulation runs representing the four types of pattern: few static hot spots (Pattern Type 1), transient hot spots (Pattern Type 2), moving hot spots (Pattern Type 3), and dense static hot spots (Pattern Type 4). The system is initialized in steady state three of the local model as indicated by  $p_3^*$  and  $s_3^*$ .



Figure 8: Changes of mean microhabitat population size when crossing the pattern formation threshold  $\chi_p^*$ . Symbols and error bars represent averages and standard deviations over ten independent simulation runs. Pattern formation commences shortly before  $\chi_p^*$  is reached and consists of four types of distinct spatio-temporal population patterns.



Figure 9: Spatio-temporal bacterial distribution (left), and mean behavior of bacterial population and substrate concentration over time (right) for a substrate diffusion coefficient 50 times lower than in other simulation runs ( $D_s = 1.8 \times 10^{-7} \text{ cm}^2/\text{s}$ ). The chemotactic sensitivity towards chemoattractant is set to a value above the pattern formation threshold ( $\chi_p = 1.99 \times 10^{-9} \text{ cm}^2/\text{s}$ ). The system is homogeneously initialized in steady state three, and all other parameters are given in Table 1.



Figure 10: Response to biostimulation (increasing K values). After an initially linear response of population density (left) and substrate consumption rate (right) to biostimulation matching steady state three of the local model  $(p_3^*)$ , biodegradation performance transiently decreases as pattern formation commences close to  $K^* = 14560$  bacterial cells. Mean over ten independent simulation runs, error bars indicate standard deviation.

\* pattern formation depends on bacterial physiology and environmental parameters

\* inhomogeneous bacterial distributions lead to reduced substrate utilization

\* onset of pattern formation leads to nonlinear response during biostimulation

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