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Modeling Population Patterns of Chemotactic Bacteria in Homogeneous Porous Media

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Abstract

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 remediation of anthropogenic contaminants. Populations of motile, chemotactic bacteria have been shown to be capable of pattern formation even in the absence of environmental heterogeneities. Focusing on the water saturated domain of the subsurface (*e.g.*, aquatic sediments, porous aquifers), we analyze this innate capability of bacterial populations in an idealized model of a homogeneous, saturated porous medium. Considering a linear array of connected, identical microhabitats populated by motile, chemotactic bacterial cells, we identify prerequisites for pattern formation, analyze types of patterns, and assess their impact on substrate utilization. In our model, substrate supplied to the microhabitats facilitates bacterial growth, and microbial cells can migrate between neighboring microhabitats due to i) random motility, ii) chemotaxis towards substrate, and iii) self-attraction. A precondition for inhomogeneous population patterns is analytically derived, stating that patterns are possible if the self-attraction exceeds a threshold defined

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

Key words: pattern formation, ecosystem services, biodegradation, chemotaxis, individual-based modeling

1. Introduction

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

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

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

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 reflected in the model.

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

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

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

$$r(s) = \mu s - d, \quad (2)$$

124 with parameter μ describing bacterial growth under maximal substrate con-
 125 centration ($s = 1$) and bacterial death controlled by parameter d . Sub-
 126 strate is supplied to the microhabitat by a generic capacitive process with
 127 rate parameter λ and consumed during bacterial growth in the microhabitat.
 128 Substrate dynamics is hence described by:

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

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

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

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

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

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

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

158 Note that the parameters D_p , D_s , χ_p , and χ_s are effective parameters that
 159 implicitly account for any flux restrictions imposed by the specific geometry
 160 of the corridors that connect neighboring microhabitats.

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

$$\begin{aligned} \frac{\partial p}{\partial t} &= D_p \cdot \nabla^2 p - \chi_s \cdot \nabla \cdot (p \nabla s) - \chi_p \cdot \nabla \cdot (p \nabla p) \\ &\quad + g(p, s) \end{aligned} \quad =: u(p, s) \quad (8)$$

$$\begin{aligned} \frac{\partial s}{\partial t} &= D_s \cdot \nabla^2 s \\ &\quad + h(p, s) \end{aligned} \quad =: v(p, s). \quad (9)$$

163 3. Model Analysis

164 3.1. Local Model

165 The local model (Equations 4 and 5) has three steady states with $g(p^*, s^*) =$
 166 0 , $h(p^*, s^*) = 0$:

$$(p_1^*, s_1^*) = (0, 1) \quad (10)$$

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

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

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

$$(p_1^*, s_1^*) : d > \mu \quad (13)$$

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

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

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

187 first two steady states are never complex, the eigenvalues for the third steady
 188 state can be complex for certain parameter settings¹, indicating oscillatory
 189 behavior. For a specific example, parameter regions with signs of eigenvalues
 190 are shown in Figure 2 for steady states two and three. The bifurcation
 191 diagram in Figure 3 illustrates how the system undergoes a transcritical
 192 bifurcation. For large values of λ , steady state two is asymptotically stable
 193 and steady state three unstable. Decreasing λ , the stability properties are
 194 switched at the bifurcation point, where saddle nodes collide with stable
 195 nodes. Decreasing λ further, a second bifurcation occurs for steady state
 196 three where the stable node becomes a stable spiral.

197 3.2. Full Model

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

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:

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

The time evolution of the perturbation d is given by

$$\begin{aligned} \frac{\partial d}{\partial t} &= Ad \\ &= \begin{pmatrix} u_p & u_s \\ v_p & v_s \end{pmatrix}_{p^*, s^*} d \\ &= \begin{pmatrix} D_p \nabla^2 - \chi_p p^* \nabla^2 + g_p^* & -\chi_s p^* \nabla^2 + g_s^* \\ h_p^* & D_s \nabla^2 + h_s^* \end{pmatrix} d, \end{aligned} \quad (17)$$

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 λ 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 λ as the eigenvalues of A . They are determined by:

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

This leads to:

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

$$a(k^2) = (D_s + D_p - \chi_p p^*)k^2 - (g_p^* + h_s^*) \quad (20)$$

$$b(k^2) = (D_p - \chi_p p^*)D_s k^4 - (D_p h_s^* + \chi_s p^* h_p^* - \chi_p p^* h_s^* + D_s g_p^*)k^2 + g_p^* h_s^* - g_s^* h_p^*. \quad (21)$$

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

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

231 Under this condition, spatial patterns can be expected.

232 4. Individual-Based Model Implementation

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

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

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

252 allows us to assign the probabilities as:

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

$$P_d := d \cdot \Delta t. \quad (25)$$

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

cell, two uniformly distributed random numbers r_μ and r_d are drawn over the interval $[0, 1]$. 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_μ 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:

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

with

$$P_0 = 1 - \frac{2D_p\Delta t}{(\Delta x)^2} - \frac{\chi_s\Delta t}{(\Delta x)^2}(s_{i+1} - 2s_i + s_{i-1}) - \frac{\chi_p\Delta t}{(\Delta x)^2}(p_{i+1} - 2p_i + p_{i-1}) \quad (27)$$

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

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

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

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

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

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

5. Simulation Results

5.1. Bacterial Growth in the Local Model

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

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

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

331 5.3. *Pattern Formation*

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

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

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

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 capacity K describes the maximum number of cells that can be supported in one microhabitat. This limit depends on microhabitat size, and can additionally also depend on further requirements for bacterial growth, for example terminal electron acceptors such as nitrate or sulfate, which are not explicitly considered in our model. Hence, an addition of terminal electron acceptors translates into an increase of K in our model. Combining the pattern formation condition Equation 22 with the condition for steady state three representing substrate limited growth (Equation 12) leads to:

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

as the condition for pattern formation. This formulation makes it evident that an increasing value of K due to biostimulation efforts can lead to the pattern formation condition to become true and hence the emergence of spatially inhomogeneous bacterial population patterns. To evaluate the resulting effect on substrate degradation as an desired ecosystem function, we perform a series of simulation runs with increasing K values and consider the mean consumption rate and mean population density over the whole array and entire simulation time, excluding the initial transient phase (Figure 10). The consumption rate is computed as substrate concentration decrease due to microbial growth (second summand in Equation 5, but without scaling factor K). Chemotactic sensitivity towards chemoattractant is set to 1.3×10^{-9} cm²/s. Under these parameter settings, the pattern formation threshold for the carrying capacity K is $K^* = 14560$ bacterial cells. The response to biostimulation can be divided into three stages (Figure 10). For low K values,

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

6. Discussion

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

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

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

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

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

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

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635 **Tables**

Table 1: Parameter values for individual-based simulations, based on typical values for *E. coli*

Parameter	Value	Reference
μ 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)
λ substrate inflow	0.004 min ⁻¹	Keymer et al. (2006)
ε conversion efficiency	0.15	Keymer et al. (2006)
D_s substrate diffusion coefficient	9×10^{-6} cm ² /s	Berg (1983)
D_p bacterial diffusion coefficient	5.19×10^{-6} cm ² /s	Berg and Turner (1990)
χ_s chemotactic sensitivity to substrate	1.3×10^{-3} cm ² /s	Berg and Turner (1990)
χ_p chemotactic sensitivity to bacteria	$1.3 \times 10^{-9} - 1.3 \times 10^{-8}$ cm ² /s	
Δx distance between microhabitats	0.005 cm	Keymer et al. (2006)
Δt time step size	1 s	

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 λ , bacterial cells consume substrate with conversion efficiency ϵ and undergo cell divisions and cell death controlled by the rate parameters μ 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 μ , 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 λ values, steady state two (p_2^*, s_2^*) is asymptotically stable, and steady state three (p_3^*, s_3^*) is unstable. When decreasing λ , 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).

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 χ_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 χ_p^* . Symbols and error bars represent averages and standard deviations over ten independent simulation runs. Pattern formation commences shortly before χ_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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