

Clustering of “active” walkers in a two-component system

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This paper investigates the agglomeration of active walkers (component A) on a two-dimensional surface, described by a potential $U(r, t)$, that determines the motion of the walkers. The walkers are able to change $U(r, t)$ locally by producing a second component B, that decreases $U(r, t)$ and which can diffuse and decompose. The nonlinear feedback between the spatio-temporal density distributions of both components results in a clustering of the walkers. The analytic description is based on a set of Langevin and Fokker–Planck equations for the active walkers, coupled by a reaction-diffusion equation for the component B. We investigate the stability of homogeneous solutions, the selection equation and an effective diffusion coefficient, which is negative in the case of the agglomeration process. Computer simulations demonstrate the time evolution of the surface potential at two different time scales: the scale of independent growth and of competition of the attraction regions. They also show the time-dependent distribution of the active walkers and spatio-temporal development of the effective diffusion coefficient.

1. Introduction

Recently, much effort has been done to study the formation of DLA (diffusion-limited aggregation)-like structures by diffusing Brownian particles (for a review, see [1]). Random walkers that stick with a certain probability to a cluster seem to be the appropriate tool to simulate the dynamics of the DLA-cluster growth, which is determined by the time scale of diffusion only.

In addition to simple DLA, there are also cases where the sticking probability may depend on local variables, which can change on a time scale comparable to diffusion, and the system is better described in terms of coupled reaction-diffusion equations [2].

We consider a special type of reaction-diffusion systems, where the particles

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are able to change the local conditions themselves, which is expressed in the term "active". In our case, it means that the particles do not just move on a surface, but also interact with it. This surface should be described by a potential $U(r, t)$, and the particles are capable (i) of recognizing and (ii) of altering this potential, e.g. by local chemical reactions. On the other hand, a change of the potential should have a feedback on the "behaviour" of the particles.

Both, motion of the particles and interaction with the potential, can be determined depending on the problems to be described and should cover a wide range of applications. Recently, the model of active walkers has been used to describe the growth of neurons in the retina [3], the dielectric breakdown in a liquid [3], or the generation of rough surfaces [4,5]. It has also been applied to the construction of path networks [6] and the simulation of foraging patterns of ants [7].

2. Assumptions for interaction of the particles

We consider a two-component model. The particles of the component A are the active walkers, moving on a surface characterized by a potential $U(r, t)$. The term "active" means that the walkers are able to interact with the surface and thus change the potential. $U(r, t)$ therefore may consist of two parts,

$$U(r, t) = U_0(r, t) + U_w(r, t), \quad (1)$$

where $U_0(r, t)$ means the background, that can change with time and can be influenced by external fields (like the environmental potential in ecology), and $U_w(r, t)$ is the part of the potential that is changed by the walker.

In order to specify this change we assume that the particles of component A constantly produce a substance of component B at a rate q [1/s] just at the place where they are:



If $b(r, t)$ denotes the surface density [particles/m²] of component B, the surface potential shall be influenced by B in the following way:

$$U(r, t) = U_0 - gb(r, t). \quad (3)$$

Here the potential U_0 is set to be constant and g means some dimensional constant [(m²/s)²M/N_A], where M is the molar mass and N_A is the Avogadro number.

We consider that B can independently diffuse at the surface with a diffusion coefficient D_b [m^2/s] and also decompose with time, where γ [$1/\text{s}$] is the reaction coefficient of the decomposition. That means, the density of B has to obey a reaction-diffusion equation,

$$\frac{\partial b(r, t)}{\partial t} = -\gamma b(r, t) + q \sum_{i=1}^N \delta(r - R_i(t)) + D_b \Delta b(r, t). \quad (4)$$

R_i means the position of the active walker number i ($i = 1, \dots, N$) (it denotes the space coordinate on the two-dimensional surface) and δ is the delta function.

The active walker prefers to turn to the local minima of $U(r, t)$ – that means to the highest value of $b(r, t)$ – but on the other hand it only produces the particles of component B. Thus we have a nonlinear feedback between the dynamics of the particles of both components A and B that reminds us of the *chemotaxis*, e.g. of ants which lay a pheromone into the ground [8] to use it for their orientation.

3. Equations of motion for the active walker

The equation of motion for the N active walkers with the positions R_1, \dots, R_N is given by the following Langevin equation:

$$v_i = \frac{dR_i}{dt}, \quad \frac{dv_i}{dt} = -\beta v_i - \left. \frac{\partial U(r, t)}{\partial r} \right|_{R_i} + \sqrt{2k_B T \beta} \xi_i(t). \quad (5)$$

β is the friction coefficient of the walker ($m = 1$), $U(r, t)$ is the potential of the surface as introduced in eq. (3), and $\xi_i(t)$ is a white random force. As is well known, for times $t \gg t_0 = 1/\beta$ the Langevin equation can be reduced to the Einstein–Smoluchowski limit [9,10]

$$\frac{dR_i}{dt} = -\frac{1}{\beta} \left. \frac{\partial U(r, t)}{\partial r} \right|_{R_i} + \sqrt{\frac{2k_B T}{\beta}} \xi_i(t). \quad (6)$$

Inserting $U(r, t)$ (eq. (3)) we get the equation of motion for the single active walker as

$$\frac{dR_i}{dt} = \frac{g}{\beta} \left. \frac{\partial b(r, t)}{\partial r} \right|_{R_i} + \sqrt{\frac{2k_B T}{\beta}} \xi_i(t). \quad (7)$$

The first part of eq. (7) describes the fact that the walker (component A) follows the concentration gradient of component B whose time dependence is given by eq. (4), whereas the second part represents the noise that keeps it moving away.

We now go from the discrete description of the single walkers of component A to the space- and time-dependent walker density $a(r, t)$ by

$$q \sum_{i=1}^N \delta(r - R_i(t)) \rightarrow qNp(r, t) \rightarrow qa(r, t), \quad (8)$$

where $p(r, t)$ means the probability density to find a walker at the point r for a given time. Since the motion of the particles of component A obeys a Langevin equation (6), for the density $a(r, t)$ the related Fokker–Planck equation holds:

$$\frac{\partial a(r, t)}{\partial t} = \frac{\partial}{\partial r} \left(\frac{1}{\beta} \frac{\partial U(r, t)}{\partial r} a(r, t) + D_a \frac{\partial a(r, t)}{\partial r} \right), \quad D_a = \frac{k_B T}{\beta}. \quad (9)$$

D_a is the diffusion coefficient of the particles of component A. The derivative of the potential is given by the gradient of the substance B, again:

$$\frac{\partial a(r, t)}{\partial t} = \frac{\partial}{\partial r} \left(-\frac{g}{\beta} \frac{\partial b(r, t)}{\partial r} a(r, t) + D_a \frac{\partial a(r, t)}{\partial r} \right). \quad (10)$$

Introducing the distribution $a(r, t)$, the reaction-diffusion equation (4) for $b(r, t)$ can be rewritten as

$$\frac{\partial b(r, t)}{\partial t} = -\gamma b(r, t) + qa(r, t) + D_b \Delta b(r, t). \quad (11)$$

Both equations, (10) and (11), have to be solved simultaneously to find the spatio-temporal distributions for the components A and B.

4. Stability analysis for homogeneous distributions

Eqs. (10) and (11) have a homogeneous solution, given by the average densities of component A and B:

$$\begin{aligned} a_{\text{hom}} &= \langle a(r, t) \rangle = \frac{N}{S} = a_0, \quad N = \int_S a(r, t) dr, \\ b_{\text{hom}} &= \langle b(r, t) \rangle = \frac{B_{\text{tot}}}{S} = b_0, \quad B_{\text{tot}} = \int_S b(r, t) dr. \end{aligned} \quad (12)$$

The surface S on which the particles move is treated as a torus; that means, it

acts like a closed system. Therefore, diffusion cannot change the total amount B_{tot} of component B, which obeys the equation

$$\frac{dB_{\text{tot}}}{dt} = -\gamma B_{\text{tot}} + qN. \quad (13)$$

Assuming the initial condition $B_{\text{tot}} = 0$ for $t = 0$, the solution of eq. (13) is given by

$$B_{\text{tot}}(t) = \frac{q}{\gamma} N(1 - e^{-\gamma t}) \xrightarrow{t \rightarrow \infty} \frac{q}{\gamma} N. \quad (14)$$

Eq. (14) means that after an initial period, given by the time

$$t = \tau \geq \frac{5}{\gamma}, \quad (15)$$

the total amount of component B in the system has reached more than 99 percent of a constant that depends on the ratio between the production and the decomposition rates, q/γ , and on the total number N of particles that produce B.

Assuming $B_{\text{tot}} = \text{const.}$, the homogeneous solution (eq. (12)) for B is then given by

$$b_0 = \frac{qN}{\gamma S} = \frac{q}{\gamma} a_0. \quad (16)$$

Let us prove now the stability of the stationary state given by eqs. (12) and (16). Therefore, we allow small fluctuations around a_0 and b_0 :

$$a(r, t) = a_0 + \delta a, \quad b(r, t) = b_0 + \delta b, \quad \left| \frac{\delta a}{a_0} \right| \sim \left| \frac{\delta b}{b_0} \right| \ll 1. \quad (17)$$

Inserting eq. (17), linearization of eqs. (10) and (11) gives

$$\begin{aligned} \frac{\partial \delta a}{\partial t} &= -\frac{g}{\beta} a_0 \Delta \delta b + D_a \Delta \delta a, \\ \frac{\partial \delta b}{\partial t} &= -\gamma \delta b + q \delta a + D_b \Delta \delta b. \end{aligned} \quad (18)$$

With

$$\delta a \sim \delta b \sim \exp(\lambda t + i\mathbf{k} \cdot \mathbf{r}) \quad (19)$$

the dispersion relation for small inhomogeneous fluctuations with wave numbers k yields

$$\lambda_{1,2} = -\frac{1}{2}[\gamma + k^2(D_a + D_b)] \pm \sqrt{\frac{1}{4}[\gamma + k^2(D_a + D_b)]^2 - k^2 D_a(\gamma + k^2 D_b) + k^2 \frac{g}{\beta} q a_0}. \quad (20)$$

For homogeneous fluctuations ($k = 0$) we obtain

$$\lambda_1 = -\gamma, \quad \lambda_2 = 0 \quad \text{for } k = 0, \quad (21)$$

expressing the conservation of the total number of active walkers and the stability of the field $b(r, t)$ for this case. On the other hand, the system is stable against inhomogeneous fluctuations ($k \neq 0$) as long as the following relation holds:

$$D_a = \frac{k_B T}{\beta} > D_a^{\text{crit}} = \frac{1}{\beta} \left(\frac{g q a_0}{\gamma + D_b k^2} \right). \quad (22)$$

Eq. (22) determines a critical diffusion coefficient of component A, below which inhomogeneous fluctuations of a certain size result in a self-collapsing behavior of the system for a given temperature. From the limit $k \rightarrow 0$ we can obtain a critical temperature T_c from eq. (22), where for $T > T_c$ the system remains stable even against large fluctuations;

$$T_c = \frac{g}{k_B} \frac{q N}{\gamma S}. \quad (23)$$

For $T < T_c$ we do not expect a homogeneous system, but the establishment of inhomogeneities in the distributions $a(r, t)$ and $b(r, t)$. This should be evaluated during the following computer simulations of the coupled kinetic equations (10), (11).

5. Results of computer simulations

Generally, the simulated "behavior" of an active walker obeys the following schedule:

1. the walker checks the local potential $U(r, t)$;
2. depending on the value of $U(r, t)$ the walker makes a decision for the next step: (a) *deterministic active walker*: it follows this decision always, (b)

probabilistic active walker: caused by the influence of noise it follows this decision only with a certain probability;

3. the walker changes the local potential depending on a special rule to be determined;
4. the walker moves (stepwise); repeat 1.

In the considered case the local potential is given by the density of component B. Since B is produced by A, the condition at $t = 0$ is

$$U(r, 0) = U_0 = \text{const.}, \quad b(r, 0) = 0 \quad \text{for all } r \in S. \quad (24)$$

The N active walkers are initially randomly distributed on the surface. Their motion is simulated on a two-dimensional hexagonal lattice with periodic boundary conditions. Since the walker makes its decision for the next step before changing the local potential, the motions of the walkers are updated sequentially; it is also allowed that a site is occupied by more than one walker.

The walker is able to recognize the potential of its six nearest-neighbor sites and to compare it with the potential value on its site; that means, it measures the local potential gradient. It then makes its decision for the next step as a probabilistic walker:

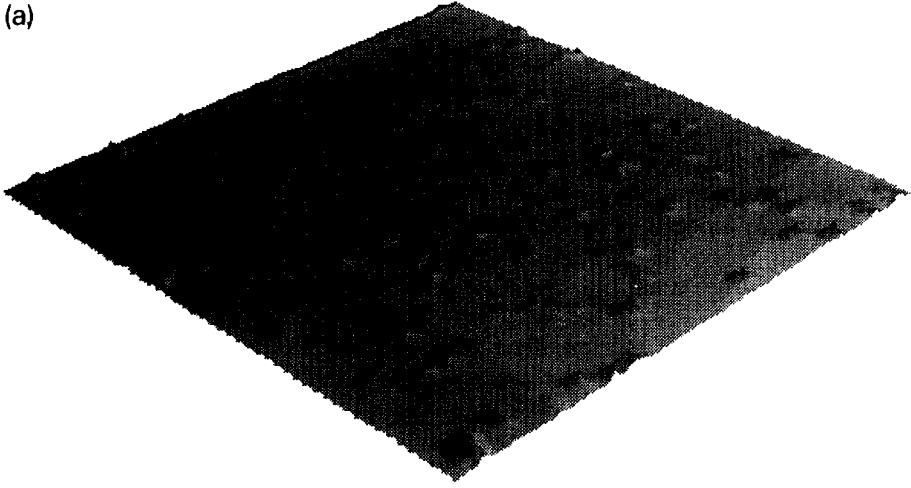
- (i) If there is no attractive potential around, it makes a random choice.
- (ii) If there is an attractive potential, it recognizes the lowest value and chooses the direction towards the minimum. But this choice is accepted only with a probability $1 - \eta$ and, with a probability η , it makes a random choice again.

Here η represents the noise in the system. Caused by the noise, the walker sometimes ignores the attraction of the potential and finds itself out of the potential minima. Since the noise keeps the walker moving, it is identified with the diffusion coefficient of the active walkers, D_a , and depends on the temperature by eq. (9). For the simulations, η is given as some portion of a critical temperature, T/T_c , where T_c is determined by eq. (23).

At every site visited the active walker produces some amount of component B and therefore decreases the local potential (eq. (3)). But, since the walker is attracted by the potential minima, this procedure involves a major problem: In most of the cases the walker should recognize the most attractive potential on the site that it has just left. This should lead to a recursive forth-and-back step cycle rather than to a move of the particle. On the other hand, the noise can push the walker out of the potential minima, which are also flattened by diffusion and decomposition of component B.

The density profile of component B (which is the negative of the potential), that results from diffusion, decomposition and from the interaction between the components A and B (eq. (11)), is presented in the time series of figs. 1 and 2. The related positions of the active walkers are shown in fig. 3.

(a)



(b)

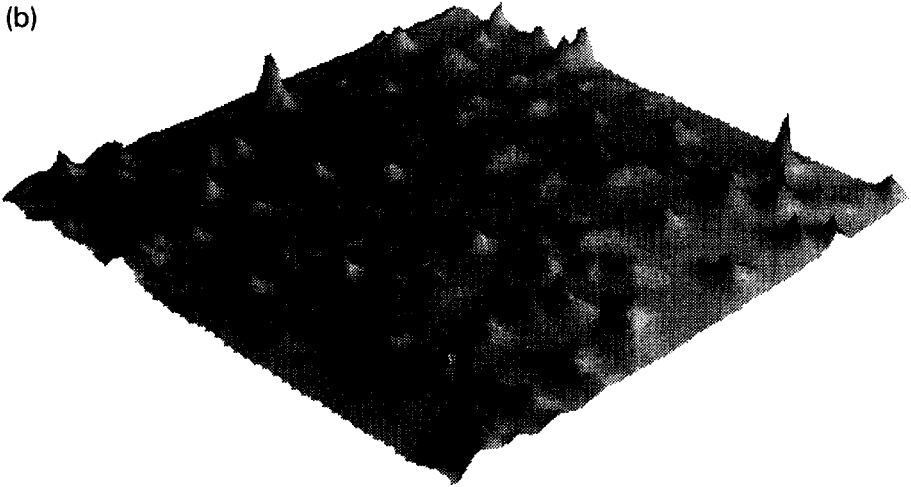


Fig. 1. Evolution of the particle density $b(r, t)$ (eq. (11)) during the growth regime. Time in simulation steps: (a) $t = 10$, (b) $t = 100$, (c) $t = 1000$. Parameters: $N = 100$, $S = 100 \times 100$, $T = 0.4T_c$ ($\eta = 0.4$), $q = 80$, $\gamma = 0.001$, $D_b = 0.01$.

For the decomposition rate, $\gamma = 0.001$, used during the simulation, we can conclude from eq. (14) that at $t = 5000$ the production of B has reached its stationary value, leading to a competitive regime for the further dynamics. Fig. 1 presents the evolution of the density $b(r, t)$ during the regime of independent growth. The random density spots, produced by the 100 active walkers in the very beginning (fig. 1a) evolve into a very jagged surface profile characterized by a reduced number of peaks of comparable height (fig. 1c) at about $t = 1000$.

(c)

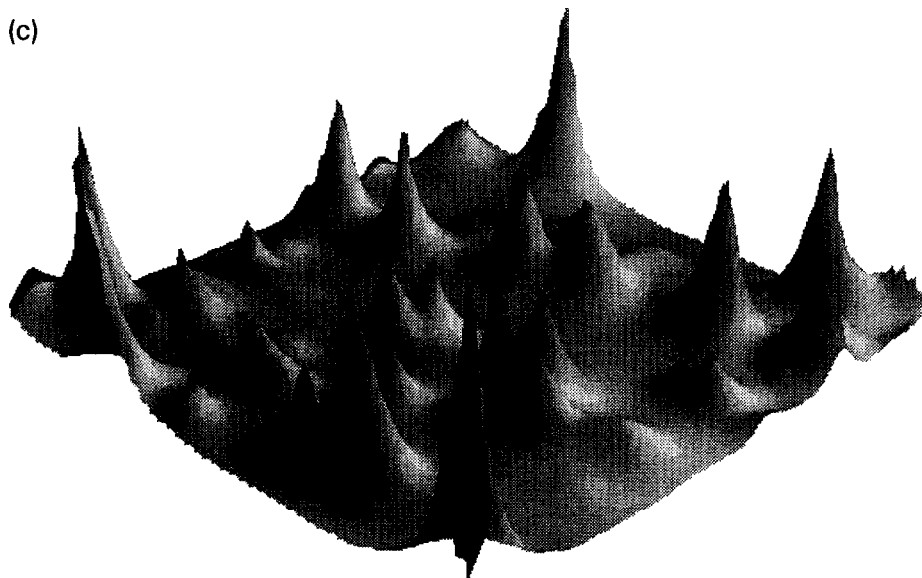


Fig. 1. (Contd.)

The same picture is seen in fig. 2a on a scale reduced by ten. Fig. 2b gives the density distribution at the beginning of the competition process, which relaxes after a long time into a one-peak distribution, as already indicated in fig. 2d. Fig 3 shows the related clustering of the active walkers. For the late stages, the positions of the large clusters are identical with the maxima of the density of component B, the distributions of which around the peaks are determined by diffusion.

6. Discussion of two quasistationary limiting cases

6.1. Derivation of a selection equation

As indicated by the computer simulations above, the spatio-temporal evolution of the densities of the components A and B follows a two-step scenario: During the initial period ($t < \tau$, where τ is given by eq. (15)), there is a nearly independent production of component B by the active walkers, leading to a nearly independent growth of the attraction areas of the potential. But, since the total amount of component B reaches a constant (eq. (14)), for times $t > \tau$, these attraction areas compete against each other for the limited amount of component B – and therefore compete for the active walkers. This necessarily leads to a selection between the most attractive areas.

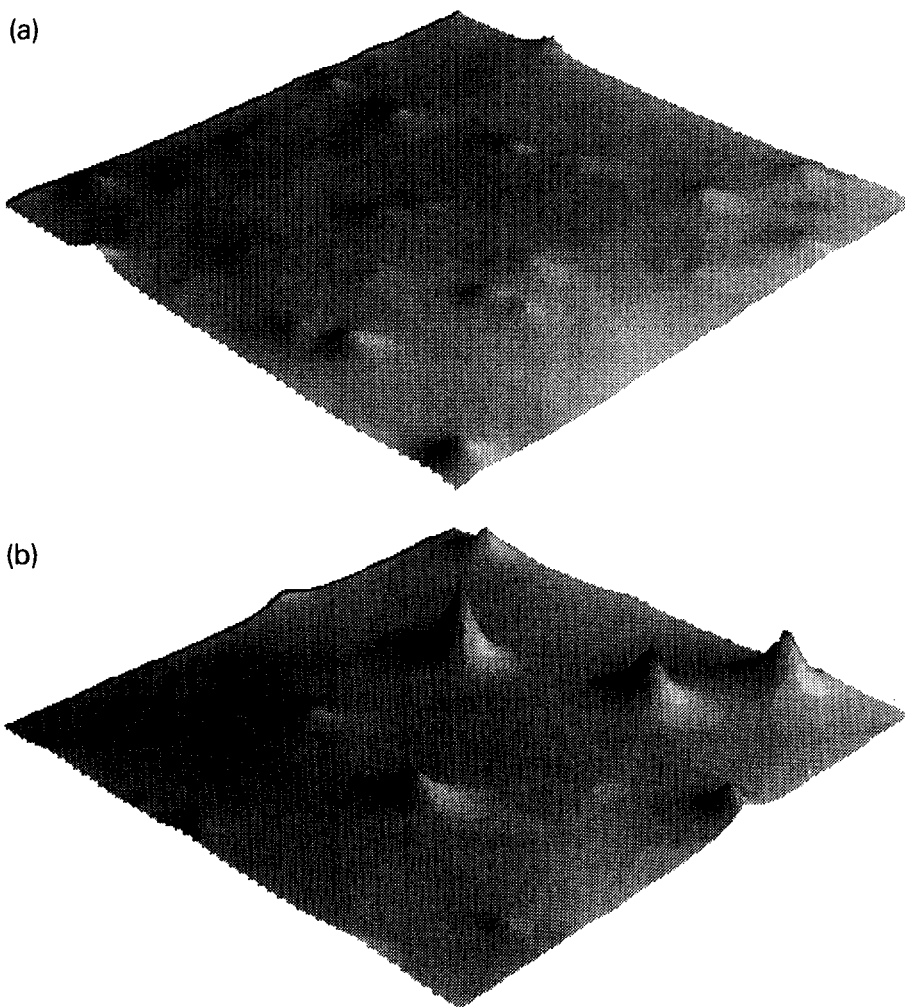
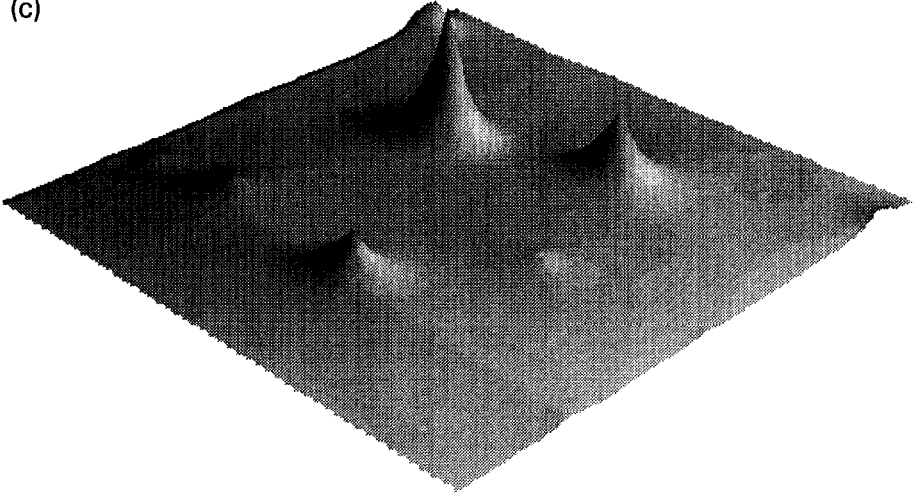


Fig. 2. Evolution of the particle density $b(r, t)$ (eq. (11)) during the competition regime. Time in simulation steps: (a) $t = 1000$, (b) $t = 5000$, (c) $t = 10000$, (d) $t = 50000$. The density scale is 0.1 times the scale of fig. 1. (a) is the same as fig. 1c and illustrates the differences of the scales. Parameters: see fig. 1.

For the further discussion of this process the reaction-diffusion equation (11) can be rewritten as

$$\frac{\partial b(r, t)}{\partial t} = \gamma b_0 \left(\frac{a(r, t)}{a_0} - \frac{b(r, t)}{b_0} \right) + D_b \Delta b(r, t), \quad (25)$$

(c)



(d)

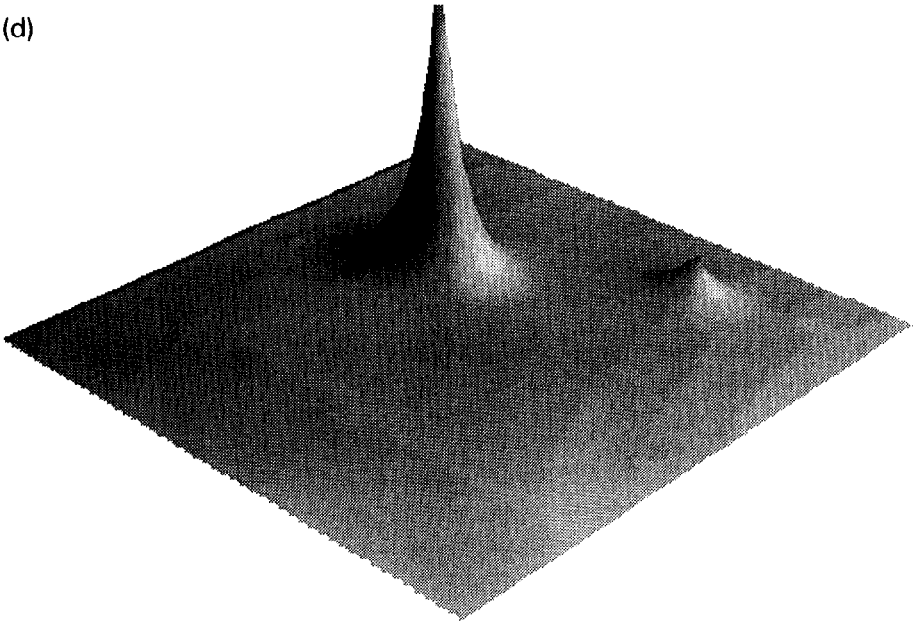


Fig. 2 (Contd)

where a_0 and b_0 are the homogeneous solutions (eqs. (12), (16)), yielded for $t > \tau$.

Let us here discuss the limiting case that $a(r, t)$ relaxes faster, compared to

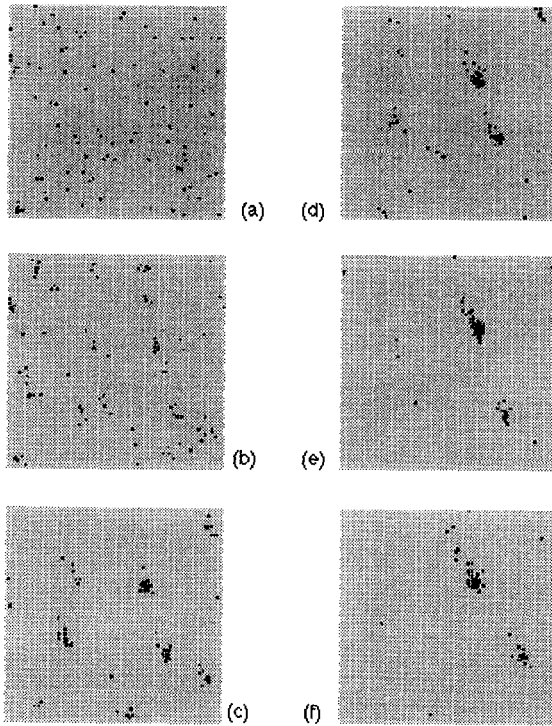


Fig. 3. Actual position of the active walkers during the simulation of figs. 1, 2. Time in simulation steps: (a) $t = 100$, (b) $t = 1000$, (c) $t = 5000$, (d) $t = 10000$, (e) $t = 25000$, (f) $t = 50000$. Parameters: see fig. 1.

$b(r, t)$, into a stationary state. The stationary solution for $a(r, t)$ results from the Fokker–Planck equation (10) via

$$D_a \frac{\partial a(r, t)}{\partial r} - \frac{g}{\beta} \frac{\partial b(r, t)}{\partial r} a(r, t) = \text{const.} , \quad (26)$$

leading to

$$a^{\text{stat}} = a_0 \frac{\exp[(g/k_B T)/b(r, t)]}{\langle \exp[(g/k_B T)b(r, t)] \rangle_S} ,$$

$$\langle \exp[(g/k_B T)b(r, t)] \rangle_S = \frac{1}{S} \int \exp[(g/k_B T)b(r', t)] dr' . \quad (27)$$

That means, in the limiting case of fast relaxation of $a(r, t)$, the density distribution of the active walkers quasistationary follows the slowly varying

distribution $b(r, t)$. After inserting $a(r, t) = a^{\text{stat}}$ (eq. (27)) into eq. (25) the time dependence of $b(r, t)$ is given by

$$\begin{aligned} \frac{\partial b(r, t)}{\partial t} = & \frac{\gamma b_0}{\langle \exp[(g/k_B T)b(r, t)] \rangle_s} b(r, t) \\ & \times \left(\frac{\exp[(g/k_B T)b(r, t)]}{b(r, t)} - \frac{\langle \exp[(g/k_B T)b(r, t)] \rangle_s}{b_0} \right) \\ & + D_b \Delta b(r, t). \end{aligned} \tag{28}$$

Neglecting the diffusion term, this equation has an obvious analogy to the selection equations of the Eigen–Fisher type (see e.g. [11]):

$$\frac{dX_i}{dt} = X_i(E_i - \langle E_i \rangle), \quad \langle E_i \rangle = \frac{\sum_i E_i X_i}{\sum_i X_i}, \tag{29}$$

where E_i is the fitness of species i and $\langle E_i \rangle$ is the mean fitness representing the global selection pressure. For the system considered here, we identify in eq. (28) the first term between the brackets as the local fitness and the second term as the global fitness. In order to guarantee a local growth of the density $b(r, t)$, the local fitness has to be larger than the global one, which depends exponentially on the total density distribution.

As a result of this process we find an increasing inhomogeneity in the density $b(r, t)$, but on the other hand the growth of the spikes (domains of high density) also leads to an increase of the global selection pressure and a slowing down of the kinetics, as indicated by the prefactor of eq. (28). This selection should result in a decreasing number of spikes and finally into the establishment of only one large peak, which is also shown in the computer simulations.

For the late stage of the selection process, where only a few large and well-separated spikes exist, eq. (28) allows an estimation of the time scale of their survival or decay. Neglecting diffusion again, the decision between growth or decay of a peak is given by the sign of the term in brackets in eq. (28).

Since in the late stage the ratio (eq. (30)) for the largest spikes has an amount of the order one,

$$\frac{\exp[g/k_B T]b(r, t)b_0}{\langle \exp[(g/k_B T)b(r, t)] \rangle_s b(r, t)} \sim 1, \tag{30}$$

we get the estimation for the growth or decay of the peaks as

$$\begin{aligned}
 b(r, t) &\sim e^{\gamma t} && \text{if } \exp[(g/k_B T)b(r, t)]b_0 > \langle \exp[(g/k_B T)b(r, t)] \rangle_s b(r, t) \\
 &&& \text{(survival),} \\
 b(r, t) &\sim e^{-\gamma t} && \text{if } \exp[(g/k_B T)b(r, t)]b_0 < \langle \exp[(g/k_B T)b(r, t)] \rangle_s b(r, t) \\
 &&& \text{(decay).}
 \end{aligned} \tag{31}$$

The estimated exponential growth and decay is, of course, modified by the diffusion of component B.

We want to underline the striking similarities of the spikes discussed here to pattern formation in active media [12]. In a similar way Mikhailov and Meinke considered gliding bugs and crawling droplets at surfaces in physico-chemical systems [13]. If, on the other hand, the growth of the spikes is limited by introducing a saturation value in the generation of the B-field, as suggested in [14], these spikes should become broad domains performing an Ostwald ripening process, similar to a case discussed in [15].

6.2. Estimation of an effective diffusion coefficient

Let us now turn to the limiting case that $a(r, t)$ relaxes slower, compared to $b(r, t)$, into a stationary state.

By introducing an effective diffusion coefficient D_a^{eff} for the particle density $a(r, t)$, the Fokker-Planck equation (10) can be written in terms of a usual diffusion equation,

$$\frac{\partial a(r, t)}{\partial t} = \frac{\partial}{\partial r} \left(D_a^{\text{eff}} \frac{\partial a(r, t)}{\partial r} \right), \quad D_a^{\text{eff}} = D_a - \frac{g}{\beta} \frac{\partial b(r, t)}{\partial a(r, t)} a(r, t). \tag{32}$$

D_a^{eff} depends on the distribution of the active walkers, $a(r, t)$ and on the relation between the densities $b(r, t)$ and $a(r, t)$. As indicated by eq. (14), for the latter only a global relation holds for $t > \tau$:

$$\int_s b(r, t) dr = \frac{q}{\gamma} \int_s a(r, t) dr. \tag{33}$$

If $b(r, t)$ relaxes faster, compared to $a(r, t)$, into its stationary state and the further discussion is restricted to the limit case of small diffusion of component B, we get instead of eq. (33) the relation

$$\frac{\partial b(r, t)}{\partial t} \approx 0 \rightarrow b(r, t) = \frac{q}{\gamma} a(r, t), \quad \text{if } D_b \rightarrow 0. \tag{34}$$

Inserting eq. (34), the effective diffusion coefficient for the particles of component A (eq. (32)) reads

$$D_a^{\text{eff}} = D_a - \frac{g}{\beta} \frac{q}{\gamma} a(r, t) = \frac{1}{\beta} [k_B T - gb(r, t)]. \quad (35)$$

We notice that the effective diffusion coefficient is not necessarily always larger than zero, which means a spreading of particles over the whole surface. It can also be less than zero, resulting in a lump of particles that keep themselves only in a certain region on the surface. Depending on the spatio-temporal density distribution $b(r, t)$, at the same time D_a^{eff} can have quite the opposite effect at different places.

6.3. Relation to nucleation theory

The results obtained from the two limit cases discussed above have an obvious analogy to nucleation theory. Selection equations like eq (28) are also found to describe the process of Ostwald ripening among clusters of different sizes, that can occur in the late stage of first-order phase transition [16].

On the other hand, we also have phase transitions, where not one single global selection parameter describes the coarsening of the system, but the growth or decay of clusters is governed by local critical parameters like the local supersaturation [17] changing with time in dependence of the interaction in the system. The effective diffusion coefficient (eq. (35)) plays the role of such a local critical parameters and, therefore, in the following it should be discussed in terms of a local supersaturation.

Considering a usual phase diagram, nucleation occurs only inside the coexistence curve, which divides the homogeneous system from the two-phases region. In our case, the phase separation is given by the agglomeration of the active walkers, and the phase separation line is defined by $D_a^{\text{eff}} = 0$, determining an equilibrium density $b_{\text{eq}}(T)$ that depends only on temperature:

$$D_a^{\text{eff}} = 0, \quad b_{\text{eq}}(T) = \frac{k_B T}{g}. \quad (36)$$

Calculating the ratio we get

$$\varepsilon(r, t, T) = \frac{D_a^{\text{eff}}}{D_a} = 1 - \frac{b(r, t)}{b_{\text{eq}}(T)}, \quad (37)$$

where $b(r, t)/b_{\text{eq}}(T) > 1$ defines the local supersaturation. For the model considered, the local production of component B leads to an increase of $b(r, t)$ and therefore, after a certain time lag, to a supersaturated state with $b(r, t) > b_{\text{eq}}(T)$. Then D_a^{eff} becomes negative and the attraction of the active walkers can occur at some critical value of the local supersaturation.

In order to determine the equilibrium value $b_{\text{eq}}(T)$ we consider the critical temperature T_c of the system, where D_a^{eff} has to be positive always, because no agglomeration occurs for $T > T_c$.

Inserting the expression for T_c (eq. (23)) into eq. (21), we get for the equilibrium density $b_{\text{eq}}(T_c)$

$$b_{\text{eq}}(T_c) = \frac{k_B T_c}{g} = \frac{B_{\text{tot}}}{S} = \frac{qN}{\gamma S}, \quad (38)$$

which occurs with the mean density of component B. This leads to the expression for the equilibrium concentration:

$$b_{\text{eq}}(T) = \frac{qN}{\gamma S} \frac{T}{T_c} = \frac{qN}{\gamma S} \eta. \quad (39)$$

We are now able to recalculate the spatio-temporal distribution of the effective diffusion coefficient $\varepsilon(r, t, T)$ (eq. (37)) within the limit that is given by the quasistationary assumption for $b(r, t)$ (eq. (34)). This is applied to the computer simulations carried out in figs. 2, 3.

In fig. 4 the black areas indicate a negative effective diffusion coefficient, leading to an agglomeration of the active walkers. We want to notice its inhomogeneous distribution. As shown, the attraction area is decreasing with time in diversity as well as in area, indicating the selection process among the attraction areas and the clustering of the walkers.

Eq. (39) also helps us to understand how a change of the decomposition rate γ or the temperature (\sim noise η) changes the agglomeration process: A larger γ increases the supersaturation, and, as is known from eq. (15), also the selection process starts earlier. This situation is shown in fig. 5, where γ is ten times larger than before. The initial situation for the simulation is the same as in the figures discussed above, but the competition starts already at $t = 500$, and the distribution of the density $b(r, t)$ as well as the effective diffusion coefficient show a much larger diversity at this time. Therefore, the whole process of selection and agglomeration of the active walkers takes a much longer time, as can be seen by comparing fig. 2d and fig. 5c, which are taken after the same number of simulation steps.

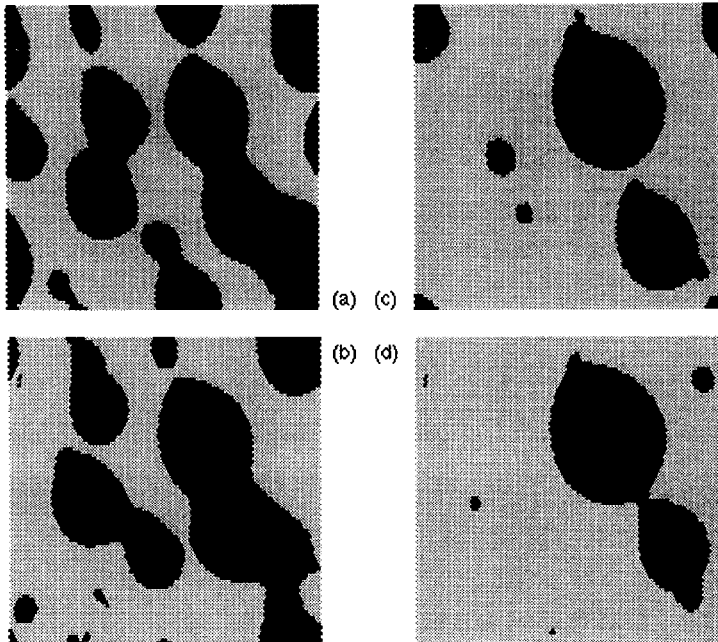


Fig. 4. Spatio-temporal evolution of the effective diffusion coefficient $\varepsilon(r, t, T)$ (eq. (22)) during the simulation of fig. 2 (competition regime). The black area indicates $\varepsilon < 0$, which means an attraction area for the active walkers; the grey area indicates $\varepsilon > 0$. Time in simulation steps: (a) $t = 5000$, (b) $t = 10000$, (c) $t = 25000$, (d) $t = 50000$. Parameters: see fig. 1.

7. Conclusions

We have discussed a two-component reaction-diffusion system. Component A is “active” in the sense, that it is able (i) to recognize, and (ii) to change the local potential, which determines its further motion. This nonlinear feedback is simulated by a chemical reaction of A, describing the production of a second component B, that can also decompose and diffuse. Since the production of B reaches a stationary value, we found a two-step scenario for the evolution of the densities: an earlier stage of independent production of B, and a late stage of competition among the B-rich areas. The related distribution of component A shows the cluster formation of the active walkers in time.

For the limiting case, where $a(r, t)$ relaxes fast into a quasistationary distribution and follows the slowly varying density of component B, a selection equation for $b(r, t)$ describes the crossover to a unimodal density distribution. If, on the other hand, the distribution of $b(r, t)$ is quasistationary compared to the change of $a(r, t)$, we found an effective diffusion coefficient for component

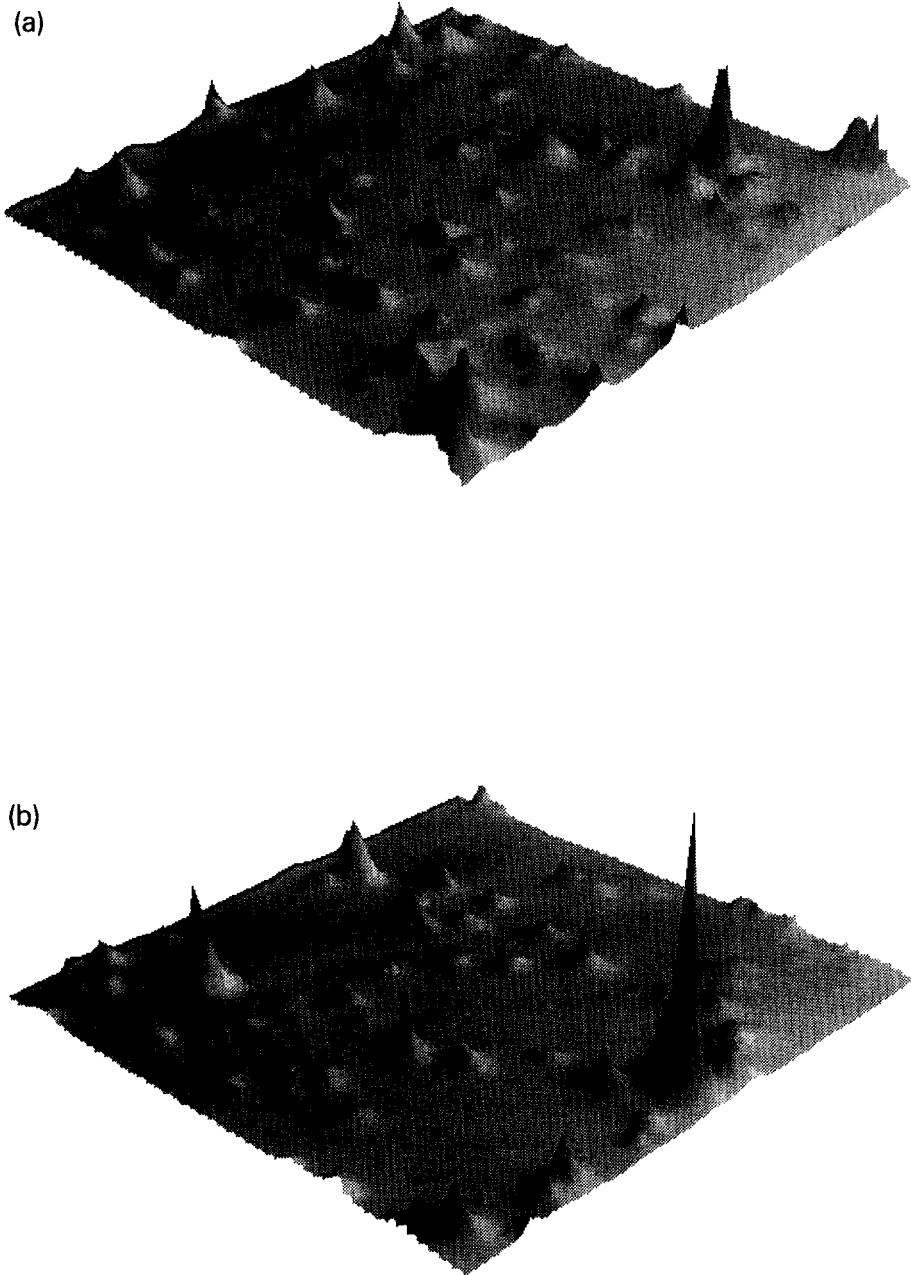


Fig. 5. Evolution of the particle density $b(r, t)$ and the related effective diffusion coefficient $\epsilon(r, t, T)$ during the competition regime for a decomposition rate: $\gamma = 0.01$ (that is ten times larger than in figs. 1–4). Time in simulation steps: (a), (d) $t = 500$; (b), (e) $t = 10000$, (d), (f) $t = 50000$. The density scale and the other parameters are the same as in fig. 1.

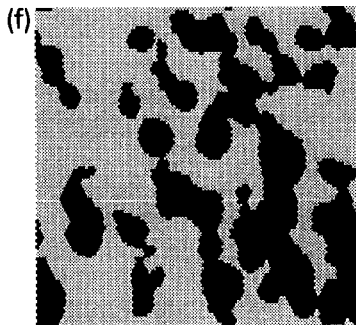
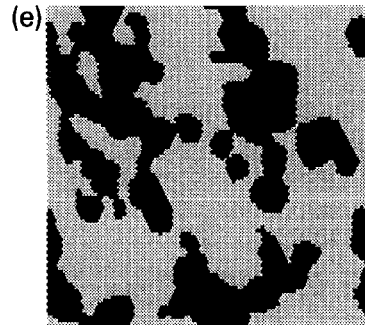
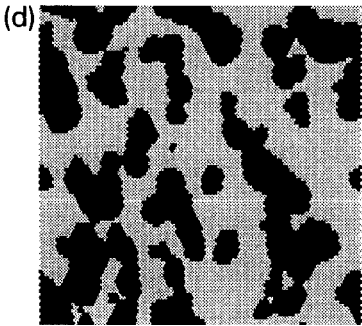
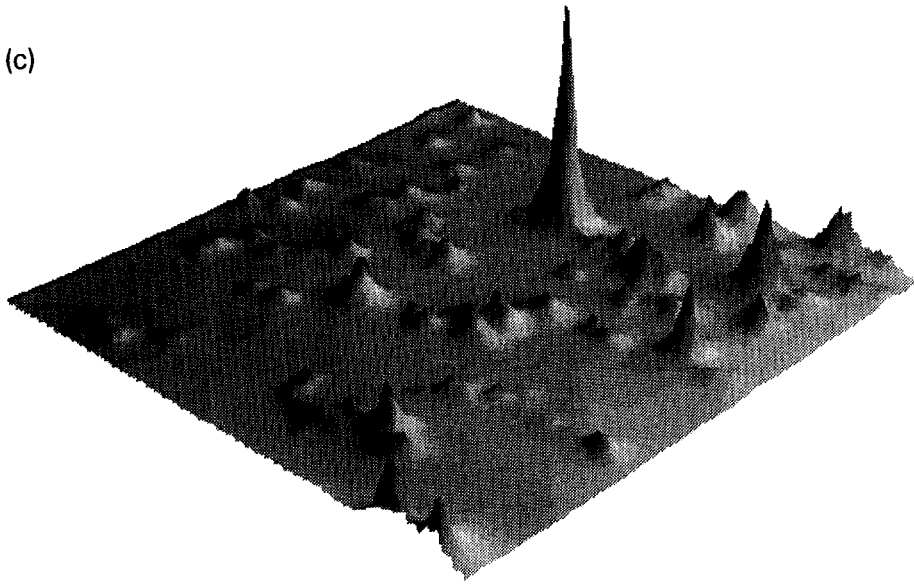


Fig. 5. (Contd.)

A that changes in space and time and can also be less than zero, leading to an agglomeration of the active walkers.

We want to point out that the basic features discussed within this paper have a range of analogies in different processes, e.g. in chemotaxis. It has been shown recently [6,7] that the same model can produce a path network as well, when applying some special conditions obtained from ants. This network also results from the interplay between the nonlinear feedback and selection, described here, and remains stable in space and time in the limit of vanishing diffusion of component B.

On the other hand, it seems that the active walker model, described here, is applicable to serve as a simple model for a communication process, that consists of three parts:

1. "writing": the walkers mark their place with a concentration;
 2. "reading": the walkers check the local concentration field;
 3. "acting": the walkers make a decision and follow the higher concentration.
- Communication is a collective process in which all walkers are involved; the information one produces affects the decisions of the other ones: it could be amplified during the evolution or disappear again.

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