

Chapter 2

Spreading Fundamentals

Armin Bunde, Christian Chmelik, Jörg Kärger and Gero Vogl

2.1 Diffusion Step by Step

Stimulated by their thermal energy, atoms and molecules are subject to an irregular movement which, in the course of history, has become known under the term diffusion. Today, in a more generalized sense, essentially any type of stochastic movement may be referred to as diffusion.

Diffusion *sensu stricto* is the motion of individual objects by way of a “random walk”. For simplicity we start with the one-dimensional problem: our random walker is assumed to move along only one direction (the x coordinate) and to perform steps of identical length l in either forward or backward direction. Both directions are equally probable and the direction of a given step should in no way affect the direction of a subsequent one (Fig. 2.1).

Such sequences of events are called uncorrelated. The mean time between subsequent steps is denoted by τ . Obviously, nobody can predict where exactly this random walker will have got to after n steps, this means, at time $t = n \tau$.

A. Bunde
Institute of Theoretical Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16,
35392 Giessen, Germany
e-mail: arminbunde00@googlemail.com

C. Chmelik · J. Kärger (✉)
Faculty of Physics and Earth Sciences, Leipzig University, Linnéstr. 5, 04103 Leipzig,
Germany
e-mail: kaerger@physik.uni-leipzig.de

C. Chmelik
e-mail: chmelik@physik.uni-leipzig.de

G. Vogl
Faculty of Physics, University of Vienna, Strudlhofgasse 4, 1090 Vienna, Austria
e-mail: gero.vogl@univie.ac.at

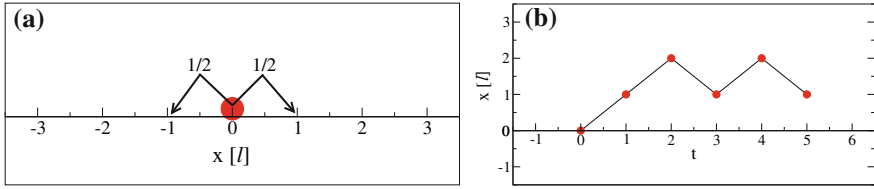


Fig. 2.1 Random walk in one dimension. **a** Step to the left and step to the right equally probable. **b** Possible displacement after five steps

The randomness of the process allows predicting probabilities only. Let us consider a large number of random walks, all beginning at the same point. The probability that at time t a random walker shall have got to position x is then simply the ratio between the number of random walks leading to this point and the total number of walks.

We are going to derive the “mean square displacement” $\langle x^2(t=n\tau) \rangle$ as a characteristic quantity of such a distribution. It denotes the mean value of the square of the net displacement after n steps, corresponding to time $t = n\tau$. Mean values are determined by summing over all values and division by the number of values considered. For our simple model we obviously have

$$\begin{aligned} \langle x^2(t=n\tau) \rangle &= \langle (x_1 + x_2 + x_3 + \dots + x_n)^2 \rangle \\ &= \langle x_1^2 + x_2^2 + x_3^2 + \dots + x_n^2 + 2x_1x_2 + 2x_1x_3 + \dots + 2x_{n-1}x_n \rangle \end{aligned} \quad (2.1)$$

where x_i denotes the length of the i -th step. The magnitude of x_i can be either $+l$ (step in $(+x)$ direction, i.e. step ahead) or $-l$ (step in $(-x)$ direction), so that all of the first n terms in the second line become equal to l^2 . Let us now consider the mean value of each of the subsequent “cross” terms $x_i x_j$, with $i \neq j$. For a given value of x_i , according to our starting assumption, the second factor x_j shall be equal to $+l$ and to $-l$ with equal probability. Hence, the resulting values $x_i x_j$, with $i \neq j$, will be equally often $+l^2$ and $-l^2$, leading to a mean value of zero.

Equation (2.1) is thus seen to simply become

$$\langle x^2(t) \rangle = n l^2 = \frac{l^2}{\tau} t, \quad (2.2)$$

with the most important message that a diffusant departs from its origin not in proportion with time as it would be the case with directed motion. It is rather the square of the displacement which increases with time, so that the (mean) distance often called x_{rms} (*rms* meaning root of the mean square) increases with only the square root of time.

Quite formally, we may introduce an “abbreviation”

$$D = \frac{l^2}{2\tau} \quad (2.3)$$

so that now Eq. (2.2) may be noted in the form

$$\langle x^2(t) \rangle = 2Dt. \quad (2.4)$$

We shall find in the subsequent section that the thus introduced parameter D is a key quantity for quantifying the rate of the random movement which we have referred to as diffusion. We may rearrange Eq. (2.4), leading to its general definition,

$$D = \frac{\langle x^2(t) \rangle}{2t}. \quad (2.5)$$

D is referred to as the self-diffusivity (or coefficient of self-diffusion or self-diffusion constant). The considerations may be extended to two and three dimensions, where the factor 2 on the right-hand side of Eq. (2.3) (and, correspondingly, in Eqs. (2.4) and (2.5)) has to be replaced by 4 and 6, respectively.

Abandoning the simplifying condition of equal step lengths, with essentially the same reasoning as exemplified with Eq. (2.1), Eq. (2.3) may be shown to be still valid, now with l^2 as the mean squared step length.

2.2 From Random Walk to Fluxes

Though today it is possible to follow the diffusion path (“trajectory”) of an individual molecule [1], the relevance of diffusion becomes more obvious if ensembles of diffusing particles are considered. This situation is schematically presented in Fig. 2.2. In the following we shall explain that it illustrates the situation typical of the three most important ways to measure and characterize diffusion. The circles represent the diffusing particles and the lattice indicates that the process occurs within some “framework” formed by, e.g. open spaces (vacancies) in a solid state lattice, interconnected pores or territorial areas, which may serve as a reference system. Correspondingly, the scheme has to be modified (see, e.g., Chap. 13 and Fig. 13.1) when diffusion of the lattice constituents (as in solid-state diffusion) is considered.

Let us start our discourse with Fig. 2.2a, with the concentration of diffusants deliberately chosen to decay from left to right. This gradient in concentrations effects that, irrespective of the random (and, notably, undirected!) movement of each individual particle, their superposition leads to a directed flux. Macroscopically, this particle flux abolishes existing concentration gradients, following the general tendency towards equilibration in nature.

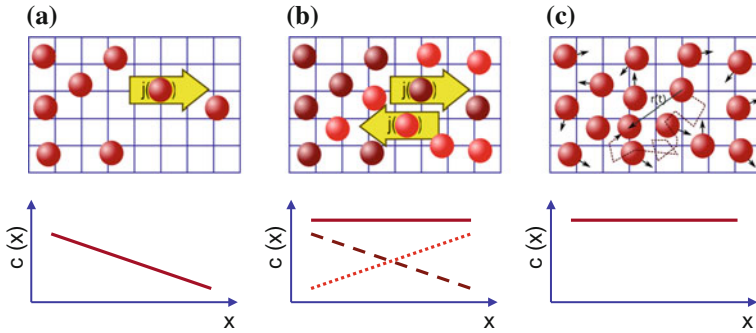


Fig. 2.2 Microscopic situation corresponding to the measurement of the transport (chemical) diffusivity **(a)** and of the self- (tracer) diffusivity **(b, c)** by either observing the flux of a labeled fraction (see e.g. [2] and Chap. 13) **(b)**, or by recording the individual displacements, e.g. by methods as PFG NMR ([3] and Chap. 12), quasi-elastic neutron scattering [4, 5], Mössbauer spectroscopy [5] or X-ray photon correlation spectroscopy XPCS [6] **(c)**. Examples of typical particle distributions on top and corresponding spatial dependencies of concentration below. Reproduced with permission from Ref. [7], copyright (2013) Wiley-VCH Verlag GmbH & Co. KGaA

Doubling the concentration gradient will obviously effect a doubling of the difference between the numbers of particles passing from left to right and from right to left and, hence, a doubling of the flux. This leads to the famous Fick's 1st law

$$j_x = -D_T \frac{\partial c}{\partial x}. \quad (2.6)$$

j_x denotes the flux density in x direction, where the x coordinate is chosen to indicate the direction of falling concentration and the index T indicates "transport". The flux density $j_x = \Delta N / \Delta A \cdot \Delta t$ is defined by the number ΔN of particles passing an area ΔA (perpendicular to the flux direction) during a time interval Δt , divided by ΔA and Δt . In Eq. (2.6), the concentration gradient is represented as a so-called partial derivative, which has to be introduced whenever a quantity (here the particle concentration c , i.e. the particle number per volume) is a function of various parameters, such as location (x) and time (t) in our case. This twofold dependence is expressed by the notation $c(x, t)$. Partial derivation means that one considers derivation with respect to one parameter (here x) while the other one(s) is (are) kept constant. The minus sign in Eq. (2.6) indicates that the particle flux is directed towards decreasing concentration. The factor of proportionality, D_T , is referred to as the coefficient of transport diffusion (as indicated by suffix T). Alternatively also the terms chemical or collective diffusion are used.

Let us return to Fig. 2.2, where we will now look for an option to quantify diffusion under equilibrium conditions, i.e. for uniform concentration. In this case, obviously, the irregular particle movement does not lead to any net flux. As illustrated by Fig. 2.2b, however, again a macroscopically observable effect may be

generated if we are able to effect a distinction between the particles of the system without affecting their microdynamic properties. In Fig. 2.2b it is simply achieved by considering spheres in two different shades of red, with both of them assumed to behave identically and the respective concentrations given below in the figure. With this distinction, again fluxes become macroscopically observable. In complete analogy to Eq. (2.6) we may note

$$j_x^* = -D \frac{\partial c^*}{\partial x} \quad (2.7)$$

where the asterisk (*) indicates that only one sort of the differently labelled particles (i.e. either the red or the pink spheres) is considered. In experiments, such a situation may be realized by using (two) different isotopes as diffusing particles. With reference to the use of labelled molecules (“tracers”), the thus defined quantity D is referred to as the tracer diffusivity. It might come as a surprise that, at the end of this section, the thus defined tracer diffusivity will be found to coincide with the self-diffusivity introduced in the previous section.

A macroscopically existing concentration gradient (Fig. 2.2a) will generally give rise to an additional bias, as a consequence in the difference in the “surroundings” depending on whether the diffusant is moving into the direction of higher or smaller concentration. The rate of propagation of the diffusants depends on the existence of “free sites” in the range where they try to get to. While in “highly diluted” systems this should not be a problem since “free sites” can be assumed to be anywhere easily (and, hence, with equal probability) available, the situation becomes more complicated with increasing density of the diffusants. This is true, e.g., for diffusing molecules if the cavities in a porous material are occupied already by other guest molecules, for diffusion in solids where generally the concentration of free sites (vacancies) is very low, or if a new generation of farmers is forced to leave their home ground in search for new farming areas, getting into even more densely populated districts.

Such type of bias does not exist in the absence of macroscopic concentration gradients (Fig. 2.2b). Hence, reflecting two different microdynamic situations, the coefficients of tracer and transport diffusion cannot be expected to coincide quite in general. We shall return to some general rules for correlating these two types of diffusivities in Sect. 2.3. Before, however, we are going to illustrate why the coefficients of self-diffusion (as introduced by Eq. (2.5) and as resulting with a measuring procedure as illustrated by Fig. 2.2c) and of tracer diffusion (Eq. (2.7) and Fig. 2.2b) are one and the same quantity.

Figure 2.2c takes us back to Sect. 2.1 with Fig. 2.1 and Eq. (2.2) illustrating the evolution of the probability distribution of diffusing particles. Now we are going to show that this very problem may as well be treated within the frame of Fick’s first law (Eq. (2.6)). For this purpose, we consider the change of the number of particles within a volume element due to diffusion. The way of reasoning is sketched in Fig. 2.3, where again we have made use of the simplifying assumption that the flux is uniformly directed into x direction (which implies uniform concentration in any

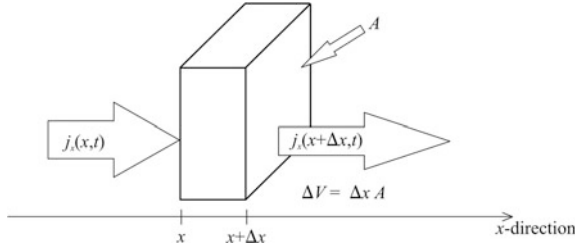


Fig. 2.3 Particle balance in a volume element $\Delta V = \Delta x \cdot A$ for diffusion in x -direction. The change in the number of particles within this volume element per time is equal to the differences of the fluxes leaving and entering. Reproduced with permission from Ref. [9], copyright (2014) Leipziger Universitätsverlag

y - z plane). For an extension to three dimensions, with the option of also orientation-dependent diffusivities, we refer to Chap. 12 and, notably, Sect. 12.5.2.

As is evident: particles entering (flux j) into a given volume must leave again or—if they do not leave again—will increase the density (c) in the volume:

$$\frac{\partial j}{\partial x} = - \frac{\partial c}{\partial t} \quad (2.8)$$

This relation is termed the continuity equation.

Inserting Eq. (2.8) into Eq. (2.6) yields

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (2.9)$$

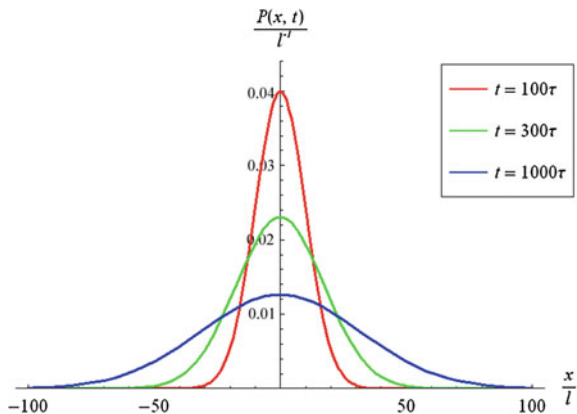
where, for simplicity, the diffusivity is assumed to be uniform anywhere in the system. Equation (2.9) represents Fick's 2nd law, stating simple proportionality between the change in concentration with time and the “gradient of the concentration gradient”, i.e. the curvature of the concentration profile. We do, moreover, disregard the suffix T having in mind that our reasoning applies to both transport and tracer diffusion.

The mathematics to treat the evolution of such a system is provided by Eq. (2.9). The reader with some background in differential calculus will easily convince himself that the function

$$c(x, t) \equiv P(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right), \quad (2.10)$$

namely a so-called Gaussian, obeys this equation (Fig. 2.4). It may be shown that, as a consequence of the central limit theorem of statistics, a Gaussian results quite generally for the distribution function of particle displacements after a sufficiently

Fig. 2.4 Evolution of the probability distribution for the end points of a “random walk” starting at $t = 0$ at $x = 0$. The curves represent the so-called probability density $P(x, t)$. Reproduced with permission from Ref. [9], copyright (2014) Leipziger Universitätsverlag



large series of uncorrelated “elementary” displacements (“steps”) if they are of identical distribution, symmetric and of finite variance, i.e. of finite mean squared “step length” (see also Sects. 3.5.1 and 4.1 and Chap. 2 in [8]). Figure 2.1 illustrated a most simple example of such a series.

With the probability distribution given by Eq. (2.10), the mean displacement can be noted as

$$\langle x^2(t) \rangle = \int_{x=-\infty}^{x=\infty} P(x, t) x^2 dx = \int_{x=-\infty}^{x=\infty} \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) x^2 dx = 2Dt, \quad (2.11)$$

which leads to a standard integral. The analytical solution yields the expression which has been given already by Eq. (2.4) where, via Eq. (2.3), D has been introduced as a “short-hand expression” for $l^2/(2\tau)$ and, by Eq. (2.5), has been defined as the self-diffusivity. This expression is now in fact seen to coincide with the tracer diffusivity as introduced by Fick’s 1st law. It was in one of his seminal papers of 1905 [10] that Albert Einstein did find this bridge between Fick’s law and random particle movement. Thus Eq. (2.5) is often referred to as Einstein’s diffusion equation. For a more profound appreciation of this achievement we refer to the presentation of “hot” Brownian motion in Chap. 8.

Diffusive fluxes in our real world are, as a matter of course, often accompanied by fluxes emerging from directed rather than from random motion. Such situations do occur in also the examples considered in our book when, e.g., diffusive fluxes in plants (Chap. 5) and turbulences in our atmosphere (Chap. 7) have to be considered in superposition with phenomena of bulk motion, referred to as advection. The combination of mass transfer by advection and diffusive fluxes is commonly referred to as convection.

Throughout the book we shall be wondering about the “driving forces” giving rise to the various types of fluxes occurring within the systems under consideration.

With Fig. 2.2. we have seen already that, under the existence of concentration gradients, diffusive fluxes emerge already as a simple consequence of random movement. In multicomponent systems of interacting particles the situation becomes more intricate. Chapter 10 gives an example that illustrates how then the gradient of the “chemical potential” may most conveniently be applied as a “driving force” of diffusion. Borrowing a conception in common use in hydrogeology, Chap. 5 deals with directed water fluxes in plants by means of Darcy’s law, with the gradient in water potential as the driving force. While thus, in physical sciences and engineering, the search for the driving forces and the quantitation of fluxes is among the tasks of today, equivalent efforts on considering spreading phenomena in e.g. humanities appear to be still far before maturity.

In problems of ecology and alike and in many problems in cultural science, spreading phenomena occur in two rather than in only one dimension as considered in our introductory example. For diffusion now $\langle r(t)^2 \rangle = 4Dt$ and again the most probable place to find a “random walker” is at the origin. As Pearson [11] put it already in 1905: “The most probable place to find a drunken man who is at all capable of keeping on his feet is somewhere near his starting point.” That is what can be seen from the cartoon Fig. 2.5 and has already been the message of Fig. 2.4 (which preserves its pattern in also two- and more-dimensional presentation): the maximum in the probability distribution of the location of a random walker remains in his starting point.

In two dimensions it is appropriate to use polar coordinates and Fick’s 2nd law is written

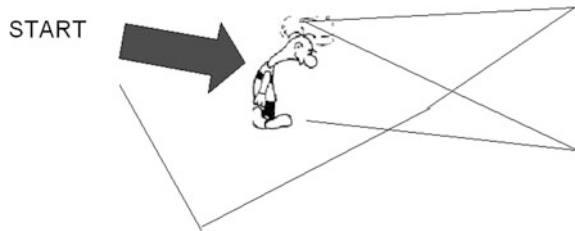
$$\frac{\partial c(r, t)}{\partial t} = \frac{D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c(r, t)}{\partial r} \right) \quad (2.12)$$

with $r = \sqrt{x^2 + y^2}$ denoting the distance between the origin of the spreading process and the considered area. Just as Eq. (2.10) resulted from Eq. (2.9), the solution of Eq. (2.12) is found to be

$$c(r, t) = \frac{n}{4\pi Dt} \exp\left(-\frac{r^2}{4Dt}\right). \quad (2.13)$$

n is the number of representatives of a certain species at the origin.

Fig. 2.5 The most probable place to find a drunken man who is at all capable of keeping on his feet is somewhere near his starting point



2.3 Interaction, Growth and Conversion

So far all our considerations were based on the simplifying assumption that the propagation probability of our diffusants is uniform all over the system under study. This implies uniformity of the medium in which the process of diffusion (spreading) occurs, as well as the absence of any interaction between the diffusants. With the lack of interaction, a distinction between equilibrium and non-equilibrium phenomena becomes meaningless [12]. The coefficients of self- and transport diffusion as considered so far do, therefore, coincide (given by Eq. (2.3) for the considered step model) and Eq. (2.9) does hold for both self- (=tracer) and transport diffusion. Due to this coincidence there was, up to this point, no real need for distinguishing between the two different types of diffusivities. On considering such interactions, however, this distinction will become necessary.

On considering molecular interactions, the diffusivity $D = D(c)$ becomes a function of the diffusant concentration c so that Fick's 2nd law is not correct anymore in the form of Eq. (2.9). Inserting Eq. (2.6) into Eq. (2.8) does now rather yield (again for the simple one-dimensional problem)

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D(c) \frac{\partial c}{\partial x} \right) = D(c) \frac{\partial^2 c}{\partial x^2} + \frac{\partial D(c)}{\partial c} \left(\frac{\partial c}{\partial x} \right)^2. \quad (2.14)$$

The particular dependence $D(c)$ of the diffusivity is determined by the system under study. Considering a variety of different types of random movement in nature, technology and society, the book presents a rich spectrum of possibilities for this dependence.

Starting with Eq. (2.8) we considered, so far, only the change in concentration of the diffusants in a certain range as resulting from in- and outgoing fluxes. On considering in particular biological species, however, we do have to consider a second mechanism, namely the generation of new species. In first order approximation this growth may be assumed to be proportional to the amount of species already present at a given instant of time. By correspondingly completing Eq. (2.12) we arrive at

$$\frac{\partial c(r, t)}{\partial t} = \frac{D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c(r, t)}{\partial r} \right) + \alpha c(r, t) \quad (2.15)$$

with the newly introduced parameter α referred to as the growth rate. By insertion into Eq. (2.15), the expression

$$c(r, t) = \frac{n}{4\pi Dt} \exp \left(-\frac{r^2}{4Dt} + \alpha t \right) \quad (2.16)$$

is easily seen to be its solution. We note that Eq. (2.16) differs from Eq. (2.13) in only the additional term αt in the exponential on the right hand side of Eq. (2.16).

This term gives rise to an increase in concentration with increasing time. For quantifying the speed of spreading we may now consider a distance R from the origin which we define by the requirement that there is a well-defined number of spreading species outside of a circle of this radius R , which is assumed to be negligibly small in comparison with their total amount. This radius R can now, as a second peculiarity, be shown to linearly increase with time [13, 14]. One finds $R(t) = 2\sqrt{Dat}$, from which the speed of spreading following what Fisher called a “wave of advance” may be noted immediately as

$$v = 2\sqrt{Da}. \quad (2.17)$$

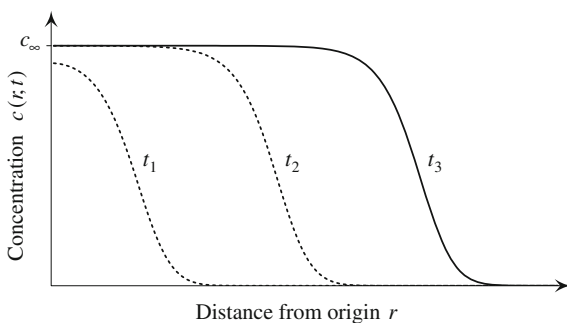
Nature does clearly forbid unlimited growth as would occur as a consequence of Eq. (2.16) as discussed above. Most remarkably, a simple correction of the term added to Fick’s 2nd law does allow a reasonable first-order description of many phenomena occurring in nature:

$$\frac{\partial c(r, t)}{\partial t} = \frac{D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c(r, t)}{\partial r} \right) + \alpha \left(1 - \frac{c(r, t)}{c_\infty(r, t)} \right) c(r, t). \quad (2.18)$$

That type of growth, eventually reaching the limiting concentration $c_\infty(r, t)$ (saturation), is termed “logistic growth”. Spreading does, correspondingly, occur with concentrations eventually arriving at the limiting concentration $c_\infty(r, t)$ as schematically shown by Fig. 2.6. The propagation rate of the concentration front (speed of spreading) is still given by Eq. (2.17). A more detailed introduction into the formalism around the “logistic growth” is provided by Sect. 3.4.

If the spreading species (as e.g. molecules during a catalytic reaction) are subject to chemical conversions or reactions, these conversions as well contribute to changes in local concentration, in addition to the influence of diffusion. Equation (2.19) gives an example of the corresponding extension of Fick’s 2nd law, Eq. (2.9), so-called reaction-diffusion equations, for sake of simplicity in the one-dimensional scenario:

Fig. 2.6 Scheme of propagation (“wave of advance”) of the concentration (number per area) of a species on spreading according to Eq. (2.17) at subsequent instants of time ($t_1 < t_2 < t_3$)



$$\begin{aligned}
\frac{\partial c_1}{\partial t} &= D_1 \frac{\partial^2 c_1}{\partial x^2} - k_{21}c_1 + k_{12}c_2 \\
\frac{\partial c_2}{\partial t} &= D_2 \frac{\partial^2 c_2}{\partial x^2} - k_{12}c_2 + k_{21}c_1
\end{aligned}
\tag{2.19}$$

for a monomolecular reaction between species 1 and 2 (of local concentrations $c_i(x, t)$ with $i = 1, 2$) with the reaction rate constants k_{ij} for conversion from j to i . For simplification, the diffusivities D_i of the two species are assumed to be independent of either concentration and the diffusive fluxes on the concentration gradient of the other component. These are coupled partial differential equations which can easily be solved by computer programmes.

The idea to use coupled reaction diffusion equations and to consider interactions in addition to growth was soon applied to the spread of living beings and even to the spread of abstract objects, in particular languages (see, e.g., Chap. 18). Already more than 30 years ago Okubo [15] and a little later Murray [16] have reported on such applications. From the considerable number of more recent applications we mention the description of diffusion (demic vs. cultural) of the Neolithic transition (see e.g. [17]) and of the spread and retreat of language [18] by coupled reaction-diffusion equations.

It is obvious, however, that one reaches limits in the analytical treatment. The subsequent sections introduce into the options how these limitations may be overcome. Now spread needs not to follow the dispersal logics of the random walk, i.e. it is not necessarily of Gaussian type.

2.4 Extending the Tools

With increasing complexity of the system, in particular of the platform on which spread occurs (network or “habitat”), it becomes increasingly complicated to obtain analytical solutions as those given by Eqs. (2.10), (2.13) and (2.16), and simple reaction-diffusion models are inadequate for the description of complex, spatially incoherent spreading patterns. The global spread of epidemics, innovations etc. are processes on a complex network. In such cases it is common praxis to rely on numerical solutions of the given equations.

When a network of starting points and destinations is the basis for the spread, for the travel of individuals between nodes n and m of the network the continuity equation $\partial c/\partial t = -\partial j/\partial x$ (Eq. (2.8)) is replaced by a rate equation

$$\frac{\partial c_n}{\partial t} = \sum_{m \neq n} (p_{nm}c_m - p_{mn}c_n)
\tag{2.20}$$

where $p_{nm}c_m$ stands for the outgoing flux from node m to node n and $p_{mn}c_n$ for the flux in opposite direction. Exactly this type of analysis we shall encounter in

Chap. 19 where Brockmann applies such network logics for demonstrating the spread of diseases [19].

Another set of interesting but complex problems are the diffusional movements of animals on search for food. For randomly distributed food sources, the Lévy flight hypothesis predicts that a random search with jump lengths following a power law minimizes the search time. Such patterns end up with relations deviating from simple proportionality between the mean square displacement and the observation time. Examples of this type of motion referred to as “anomalous diffusion” may be found in Chaps. 4 (“Levy flights”), 6 (diffusion in brain “interstitials”) and 10 (“single-file” diffusion).

However, Lenz et al. [20] find for bumblebees that the crucial quantity to understand changes in the bumblebee dynamics under predation risk, when the insects obviously try to avoid meeting predators, is the correlation of velocities v . These correlations correspond exactly to the sums of cross-terms in Eq. (2.1), which for the bumblebees do not cancel out. The authors reproduce these changes by a Langevin equation in one dimension adding a repulsive interaction U of bumblebee and predator:

$$\frac{\partial v(t)}{\partial t} = -\eta v(t) - \frac{dU}{dx} x(t) + \xi(t) \quad (2.21)$$

where η is a friction coefficient and $\xi(t)$ a fluctuating force (Gaussian white noise).

2.5 Agent-Based Models of Spread

An alternative possibility of modelling and eventually predicting spreading under complex conditions is Monte Carlo simulation on the basis of cells occupied by diffusants, so-called agents, which can be men, animals, plants, bacteria or even abstract concepts as e.g. innovations and ideas. The method is sometimes called cellular automaton. This has e.g. been done in ethnology for the spread of agriculturalists in the neolithicum [21], in ecology for the spread of neobiota [22] and in linguistics [23] for language competition, just to give a few examples.

The idea of Monte Carlo simulations is as follows: One reserves, in the computer, a sufficiently large number of memory cells designated i . These cells refer to the possible positions of the random walker introduced in Sect. 2.1. One considers a set of numbers $m_{i,j}$ which indicate the occupation number of cell i after time step j .

In the introductory example (Fig. 2.1), after each time step (of duration τ) the random walker was required to definitely step to one of the adjacent sites. Thus, one half of the given population of a certain cell (of number i) would have to be passed, after one step, to the next one (to cell number $i + 1$), the other to the previous one (cell number $i - 1$). In our computer simulation this would correspond to the relation

$$m_{i,j+1} = \frac{1}{2} m_{i-1,j} + \frac{1}{2} m_{i+1,j} \quad (2.22)$$

correlating the cell populations after subsequent steps. After 100, 300 and 1000 steps one would arrive at the occupation distributions as shown in Fig. 2.4 (where the values given in Fig. 2.4 have to be additionally multiplied by the number of agents starting at the origin).

We may come closer to the reality of the elementary steps of propagation by a modification of the simulation procedure. Rather than rigorously requiring that, after each time step τ , the agents have to definitely jump to one of the adjacent sites, one may introduce the probability $p_{i,k}$ that, during one time step, an agent gets from site k to i . This probability may include the suitability of the cell. In this case, Eq. (2.22) is replaced by a relation of the type

$$m_{i,j+1} = m_{i,j} + \sum_k m_{k,j} p_{i,k} - m_{i,j} \sum_k p_{k,i} \quad (2.23)$$

where the terms appearing on the right hand side, in addition to the given occupation number $m_{i,j}$, are easily recognized as population increase of cell i by agents entering from other cells k and population decrease by agent transfer from cell i to other ones.

With k equal to $i - 1$ and $i + 1$ and $p_{i,k} = \Delta t / 2\tau$, during a time interval Δt , an agent will leave the cell with the probability $\Delta t / \tau$, with equal probabilities for both directions. This probability definition serves as a meaningful definition of a mean residence time τ .

The need for computer simulations is illustrated with the representation in Fig. 2.7, which refers to the spreading of a biological species, namely ragweed (*Ambrosia artemisiifolia*), a plant which has “invaded” from North America and continues to enhance its density of occurrence in Europe [22].

In the top of the figure cells populated by ragweed are shown in black. The number of cells in black will continuously increase with spread of ragweed. The simulations aim at determining the probability by which, at further instants of time, so far unpopulated areas shall become populated (“infested”). In the starting assumption that infested cells remain infested, one notably deviates from the situation considered with the introductory random walker example. In fact, by considering infestation spreading, one is already following the situation typical of growing populations as considered in Sect. 2.3.

A successful step of “spreading” (the probability of which has been just considered) is not automatically assumed to warrant infestation. In fact, environmental conditions (“habitat suitabilities”) might be quite different leading to different survival probabilities. The grid on bottom left provides the numbers considered to be relevant for the given example. The products of both probabilities, representing the “total infestation probabilities” are given on top in the middle. Whether

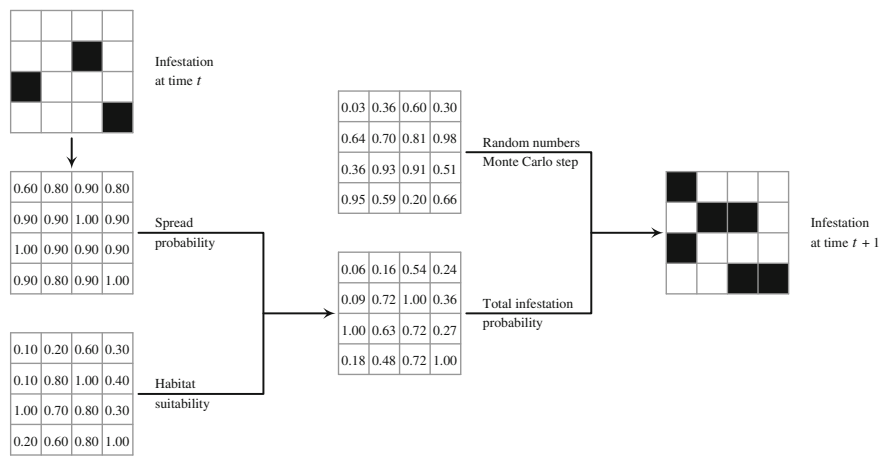


Fig. 2.7 Algorithm for determining the occurrence of a species in space at subsequent instants of time. The 4×4 squares (“grid cells”) symbolize the different areas into which the space is subdivided. Redrawn from [22]

infestation will indeed occur depends on the relation between the random numbers (between 0 and 1) produced by the computer and the total infestation probabilities. Correspondingly, in the top right grid do all these cells appear in black for which the random number is exceeded by the total infestation probability.

Figure 2.8 shows as example the predicted infestation of grid cells (about 5 × 5 km) by the spread of ragweed over Austria and Bavaria.

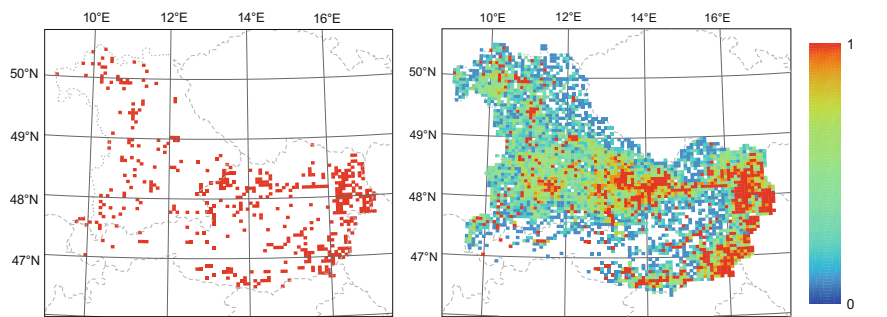


Fig. 2.8 Left: Distribution of ragweed in Austria and Bavaria in 2005. Red squares symbolize infested grid cells. Right: Predicted infestation probability indicated by colors from red (highest probability) down to blue (lowest probability) in 2050, if no action against ragweed spread is taken. Redrawn from [24]

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