Computer Simulation of Single-File Transport

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Abstract. A stochastic model of single-file transport was developed as the Markov process in continuous time technique. The model was constructed using an EC-1060 computer. Unidirectional fluxes were investigated and populations of channels were correlated with flux fluctuations. The profiles of channel populations were shown to have nonlinear shapes even with the transport of nonelectrolyte (the classical diffusion approach gives linear profiles). The relationship between the paired correlation function $F(AB)$ and the concentration of transported particles was examined. The $F(AB)$ profile was shown to become flattened (or exponential for ansymmetrical cases) at high concentrations. The concentration dependence j_A/j_A^0 ratio were analyzed, where j_A is a single-file unidirectional flux, j_A^0 is unidirectional flux for the case of free diffusion. An interesting "stack" phenomenon was observed for abnormal time correlations of single-file fluxes.

Key words: Computer simulation – Single-file transport – Unidirectional fluxes

Introduction

It is typical of the single-file transport that particles moving through a narrow pore or a channel cannot "outrun" each other. Such a simple, as would appear, restriction results in considerable modifications of transport characteristics in such systems as compared to the characteristics based on the classical description (free diffusion and migration of particles) (Goldman 1943). A significant role in single-file transport systems is played by effects, such as competition for a vacant site within the channel, correlations of channel populations, etc.

The development of the single-file transport theory may conventionally be divided into two phases: analytical methods and computer simulations methods. In the analytical phase the single-file transport was considered as a series of successive jumps over a system of potential wells and barriers. (Heckman 1965; Aityan and Chizmadzhev 1973b, 1977; Markin and Chizmadzhev 1974; Kohler and Heckman 1979). In the so-called "discrete" approach a total channel state function was considered and a balance equation for this function was constructed (Heckmann 1965; Aityan and Chizmadzhev 1973b; Markin and Chizmadzhev 1974). To solve

the problem, a very convenient diagram technique has been developed (Hill 1966; Aityan and Chizmadzhev 1977) which allows to considerably simplify calculations. However, due to some calculations problems the discrete approach has been efficient when the system included a small number of barriers (Heckmann 1965; Aityan and Chizmadzhev 1973b, 1977; Markin and Chizmadzhev 1974). For higher number of barriers it has been practical in some special cases only (Kohler and Heckmann 1979). For long channels, with a great number of barriers, the so-called "continuous" approach has been more convenient. It has been based on modifications of the classical electrodiffusion approach considering single-file effects (Aityan and Chizmadzhev 1973a, 1981; Chizmadzhev and Aityan 1982; Aityan 1985). In the continuous approach, the basic equations for the flux contained, in addition to the unitary correlation function (the population of a given well), high-order correlation functions. Even for the case of uncharged particles this equation involved the paired correlation function (Aityan and Chizmadzhev 1981; Chizmadzhev and Aityan 1982; Aityan 1985). To close the problem equations for the high-order correlation functions which obviously incorporate higher-order correlation functions should also be introduced. Usually, such a chain of equations is closed by expressing the high-order correlation functions in terms of the low-order ones. In the papers by Aityan and Chizmadzhev (1981), Chizmadzhev and Aityan (1982) and Aityan (1985) the paired correlation function was represented in a superposition approximation, namely, as the product of unitary functions. Obviously, such a description was approximative, and the question arose as to the limits of its applicability and the adequacy of such a representation.

The computer simulation methods, based on a direct construction of the physical model under consideration, are alternative approaches. These methods include the molecular dynamics method (Fisher et al 1981; Aityan and Chizmadzhev 1982, 1984, 1986) which integrates directly the equations of motion of all particles with the inclusion of their interaction, and the stochastic methods based on the theory of random processes (Aityan 1983).

In the present study we used the stochastic method of computer simulation. We considered transport through a single-file channel as a series of succesive jumps of particles over a system of potential wells and barriers (Fig. 1) according to the theory of absolute reactions rates. According to the latter theory, a particle presenting in a potential well "waits" for thermal fluctuation sufficient for its overcoming the energy barrier. By applying the corresponding law of distribution of thermal fluctuations, all the characteristics of the transport process can in principle be calculated. Since this approach is devoid of restrictions introduced in the analytical approach (Aityan and Chizmadzhev 1973a, 1981; Chizmadzhev and Aityan 1982; Aityan 1985), it gives exact results within the framework of the adopted physical representations of transport process, and the

results obtained by this method may serve as a criterion of applicability of a certain analytical approach.

Formulation of the problem

The channel structure is imagined as a series of potential wells and barriers (Fig. 1). In such a case all the rate constants of the jumps $\nu_{n,n+1}$; $\nu_{n,n-1}$ are given describing the probability densities of a jump from the well n to the well $n+1$ or $n-1$.

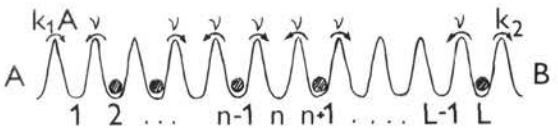


Fig. 1. Energy of the channel — a system of potential wells and barriers; possible jumps in certain situations within the channel.

The main objective of the present study was to examine the single-file transport and to elucidate the nature of the single-file transport process. Similarly as in the previous paper (Aityan 1985), we shall therefore deal with the simple case of transport of uncharged particles within a homogeneous channel (i.e. all the constants of jumps inside the channel are identical). On the left edge of the channel there is a pool containing particles A (with a concentration C_A) and no particles B, while on the right, there are particles B (with a concentration C_B) and no particles A. We shall suppose that the boundary wells of the channel are at equilibrium with the corresponding pool, i.e.

$$\theta_A(1)=\frac{\gamma C_A}{\gamma C_A+1};\ \theta_A(L)=0;$$
$$\theta_B(1)=0;\ \theta_B(L)=\frac{\gamma C_B}{\gamma C_B+1} \tag{1}$$

where $\theta_A(1)$, $\theta_B(1)$ are the probabilities of the occurrence of particles A and B in well. No. 1, and $\theta_A(L)$, $\theta_B(L)$ are the corresponding probabilities relative to the last well L; and γ is the partition coefficient. We assume as earlier (Aityan 1985) that particles A and B are different tracers of the same substance, i.e. they have identical kinetic parameters. As a result of the equilibrium population of the boundary wells (see Eq. (10)) the rate constants of the transitions for them are modified

$$\nu_{1,2}=\nu\theta_A(1) \qquad \nu_{2,1}=\nu(1-\theta_A(1))$$
$$\nu_{L,L-1}=\nu\theta_B(L) \qquad \nu_{L-1,L}=\nu(1-\theta_B(L)) \tag{2}$$

Using the method described in the preceding section, we calculated the stationary kinetic characteristics of the transport process, such as unidirectional and total fluxes, channel population profiles, paired correlation functions etc. The stationary characteristics were obtained by averaging all the iterations of the computer run.

The simulation procedure

For each specific pore state we constructed a total field of all possible transitions in the form of a straight line segments composed of segments of length $\nu_{n\pm1}$ for each possible transition in a given state of the channel. The total field of possible transitions contains no transitions incompatible with the given state. For example, if there are particles in both the n-th and $(n+1)$th well then a transition between these wells is impossible and is hence not included in the total field of transitions. On the total field of transitions we drop a random uniformly distributed number indicating the forthcoming assuming of the channel state etc. The algorithm thus follows the Markov process. However, the question arises concerning time quantitation of the process. Taking any finite discrete time step Δt two or more events may always occur simultaneously; this introduced additional problems associated with the competition of various processes since no more than one particle can be present in one well. "Replaying" of competitive situations within the framwork of a discrete time step Δt results in considerable complications of the algorithm. For example, in the situation illustrated in Fig. 1, the competition for getting into well n from wells $n-1$ and $n+1$ results in a multiple additional revision of random jumps. If we attempt to decrease the probability of the occurrence of a competitive situation by decreasing the step Δt, then the time of the computer run shall appreciably increase.

In the present paper we propose an algorithm with time being a continuous variable; consequently no problems associated with competitive situations arise. The principle of the method lies in the fact that for each state of the system a random expectation time for getting to the next state is calculated, i.e. the time during which the system does not change its state. We shall denote the total field of possible transitions for the given realization Ω.

$$\Omega = \sum_{\lambda} \alpha_\lambda \nu_\lambda \tag{3}$$

where ν_λ is the rate constant of all possible transitions in the system, and

$$\alpha_\lambda = \begin{cases} 1 & \text{if the transition is allowed in the given realization;} \\ 0 & \text{if the transition is forbidden in the given realization.} \end{cases}$$

Then, the probability of the realization of a transition in the assembly of all possible transitions is

$$P_\lambda = \alpha_\lambda \nu_\lambda / \Omega \tag{4}$$

and the probability that no transition will occur during the time t is

$$p_0 = e^{-\Omega t} \tag{5}$$

It thus appears that the probability of realization of a transition in a time interval t to $t + dt$ is

$$dP_t = \Omega e^{-\Omega t} dt \tag{6}$$

or, integrating Eq. (6) over $t \in (t, \infty)$ we obtain

$$p_t = e^{-\Omega t} \tag{7}$$

With known probabilities (4) and (7) we can simulate the transitions using a generator of random numbers $\langle S_i \rangle$ uniformly distributed in the segment 0,1.

The realization of the transition is accomplished by two random numbers S_1 and S_2. By association of the first random number with the expectation probability.

$$p_t = S_1 \tag{8}$$

we yield the system expectation time

$$t = -\frac{1}{\Omega} \ln S_1 \tag{9}$$

This means that during the time interval t the system state does not change and at the end of this time interval certain transition occurs. The realization of a transition is found by dropping the random number S_2 on the normalized field of possible transitions (3) and (4). Let us determine the monotonic function

$$f_\lambda = \sum_{\mu=1}^{\lambda} p_\mu, \quad 1 \leqslant \lambda \leqslant \Lambda; \quad f_0 = 0 \tag{10}$$

where Λ is number of all the transitions allowed in the given realization. If the random number S_2 is within the region

$$f_{\lambda-1} < S_2 \leqslant f_\lambda \tag{11}$$

then we shall suppose that the transition λ, described by the transition constant ν_λ, is realized.

Thus, each iteration of the algorithm consists in the realization of two random events. The first event is the calculation of the random expectation time t, according to Eq. (7), and the other is the realization of a random transition according to Eqs. (3) and (4). This is then repeated for the following iteration. The number of iterations is determined by the stabilization of characteristics such as

fluxes, population profiles, paired correlation functions etc., calculated at the required accuracy.

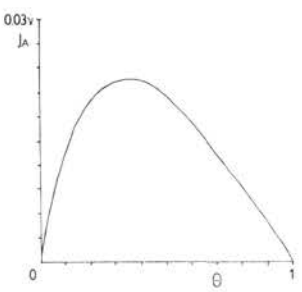
Results of Computer Simulation

The number of iterations in computer simulation was selected to obtain accuracy of the results in the order of 10^{-2} to 10^{-3}; this required $10^5$to 10^7 iterations depending upon the system parameters. The minimum number of iterations was required at a moderate population of the channels. At low and high populations the required number of iterations was increased. The number of wells within the channel was usually taken to be 10. In some instances, e.g. in examining the relationship between fluxes and number of wells, the number of wells was varied (as specified in respective considerations).

Along with the description of the results obtained by computer simulation, a comparison was made with the theoretical calculations by Aityan (1985).

Symmetrical case $C_A = C_B$

First we shall consider the case where the concentration of particles A in the left pool is equal to that of particles B in the right pool. In this case, the total flux in the system is zero and unidirectional fluxes j_A and j_B are equal in magnitude and opposite in direction. The dependence of the flux j_A on the value of the population of the boundary wells $\theta_A(1)$ (at $\theta_A(1) = \theta_B(L)$) is shown in Fig. 2. Fig. 3 also shows the relationship between the ratio of j_A to j_A^0 for diffusion without restrictions imposed by the single-file nature of the transport. It is evident from these figures that, for free diffusion at a low population θ the unidirectional flux j_A increases with increasing θ and is slightly different from the flux j_A^0, and at high population θ



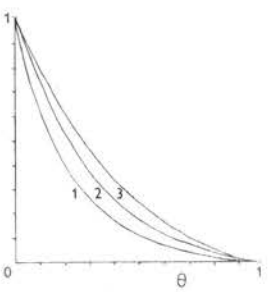


Fig. 2. Relationship between unidirectional flux and the channel population under symmetrical conditions ($\theta_A(1) = \theta_B(L)$).

Fig. 3. Relationship between the ratio of unidirectional flux to unidirectional flux, j_A for free diffusion and the channel population under symmetrical conditions. The number of wells within the channel is (1) 15; (2) 10; (3) 7.

in contrast to j_A^0 the unidirectional flux j_A decreases with increasing θ, because this flux is already determined by the transport of holes and not is that of particles. With increasing numbers of wells the dependence of the ratio j_A/j_A^0 on the channel population becomes steeper (Fig. 3).

Fig. 4 shows the profiles of populations θ_A, θ_B and the paired correlation function $F(AB)$ which determines the probability of the occurrence of particles A and B in the adjacent wells n and $n+1$. As has been demonstrated in Aityan and Chizmadzhev (1981) and Aityan (1985), the paired correlation function $F(AB)$ plays an important role in the description of the single-file transport. It is clear from Fig. 4 that at a moderate population $\theta = \theta_A + \theta_B \sim 0.5$ (Fig. 4*B*) the profiles of the populations θ_A and θ_B have a non-linear form while the profile $F(AB)$ is bell-shaped, and adequately approximated by the product of populations θ_A and θ_B in the corresponding wells; this is consistent with the assumption concerning the superposition approximation $F(AB) = \theta_A\theta_B$ (see Aityan and Chizmadzhev 1981; Aityan 1985). At a low population θ (Fig. 4*A*) the profiles θ_A and θ_B become linear similarly as in free diffusion, and fluxes j_A and j_B are equal to fluxes j_A^0 and j_B^0 obtained for free diffusion (Fig. 3); this is in agreement with the results obtained by Aityan and Chizmadzhev (1981) and Aityan (1985). Because of large fluctuations at low populations, the curve $F(AB)$ shows a rather large dispersion. At a high population (Fig. 4*C*) the profiles θ_A and θ_B are nonlinear but have nearly linear regions in the centre of the channel, and the profile $F(AB)$ differs from the product $\theta_A\theta_B$, and is flattened in the central part of the channel. In this case, unidirectional fluxes are much less than those in free diffusion, i.e. $j_A/j_A^0 \ll 1$. Figs. 5 and 6 show

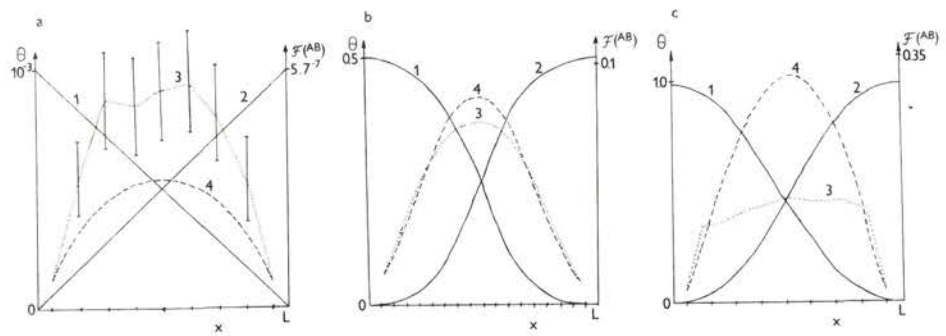


Fig. 4. Profiles of the channel population ((1) – θ_A; (2) – θ_B), the pair correlation function $F(AB)$ – (3) and the model correlation function in the superposition approximation $F(AB) = \theta_A \cdot \theta_B$ (4). Symmetrical conditions $\theta_A(1) = \theta_B(L) = \theta$ (*a*) low population, $\theta = 0.001$: because of the very low probability of the occurrence of the pair state (AB), curve (3) has a wide spread. (*b*) moderate population $\theta = 0.5$. (*c*) high population $\theta = 0.99$.

the profiles θ_A (θ_B have symmetrical profiles) and $F(AB)$ for various populations of the channels $\theta = \theta_A + \theta_B$.

Thus, comparing the results of computer simulation with the results obtained by Aityan and Chizmadzhev (1981) and Aityan (1985) who assumed in their analytical calculations the superposition approximation $F(AB) = \theta_A \theta_B$ we can say that this approximation quantitatively describes the unidirectional fluxes j_A and j_B at low moderate populations, and that at high populations, it only gives qualitatively correct trends for the flux. The paired correlation functions $F(AB)$ are correctly described by the approximation $F(AB) = \theta_A \theta_B$ (Aityan and Chizmadzhev 1981; Aityan 1985) in the region of a moderate population only; at low and high populations this approximation is incorrect. This seems to be due to the fact that, at moderate concentrations, the number of the degrees of freedom of the system is large and therefore a local equilibrium is rapidly reached at each point of the channel. However, in the region of low θ the inaccuracy of the approximation $F(AB) = \theta_A \theta_B$ does not affect unidirectional fluxes since the paired correlation function is so small that it does not influence the transport process.

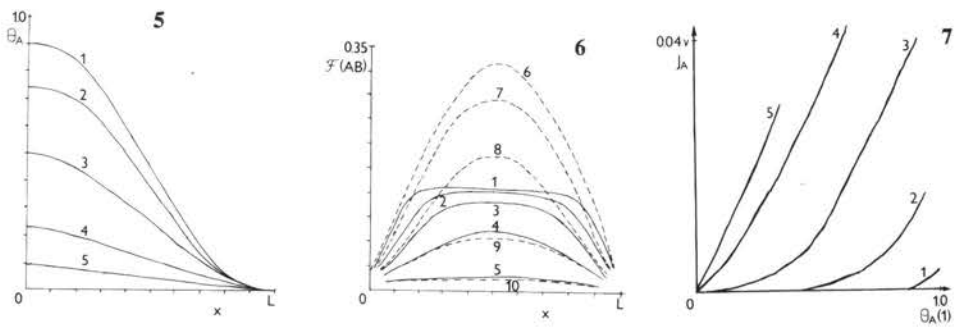


Fig. 5. Profiles of population $\theta_A(x)$ under symmetrical conditions. (1) $\theta = 0.91$, (2) $\theta = 0.75$, (3) $\theta = 0.5$, (4) $\theta = 0.23$, (5) $\theta = 0.09$.

Fig. 6. Profiles of the pair correlation function $F(AB)$ (Fig. (1—5)) and the model correlation function in the superposition approximation (Fig. (6—10)) at various populations θ. Symmetrical conditions. (1), (6) $\theta = 0.99$, (2), (7) $\theta = 0.91$, (3), (8) $\theta = 0.75$, (4), (9) $\theta = 0.5$, (5), (10) $\theta = 0.23$.

Fig. 7. Relationship between unidirectional flux j_A and the population θ_A in the left boundary well for different values of θ_B in the right boundary well: (1) $\theta_B(L) = 0.090915$; (2) $\theta_B(L) = 0.2315$; (3) $\theta_B(L) = 0.5$; (4) $\theta_B(L) = 0.8333$; (5) $\theta_B(L) = 0.9091$.

Asymmetrical case $C_A \neq C_B$

Fig. 7 shows unidirectional fluxes as functions of the population of boundary wells $\theta_A(1)$ and $\theta_B(L)$. The figure suggests that unidirectional fluxes are strongly dependent on populations. At $\theta_A(1) < \theta_B(L)$, the counterflux of particles

B severely suppresses the flux j_A. At $\theta_A(1) > \theta_B(L)$ it makes up a significant proportion of the total flux and its dependence on the population is linear. It is worth noting that the relationships shown in Fig. 7 qualitatively agree with the approximate dependences calculated in the superposition approximation of correlators (Aityan 1985). The shape of the population profiles are shown in Fig. 8. It is evident from Fig. 8 that at a superlow population (Fig. 8*A*) the population profile is linear with high accuracy, because in this case, the probability of coexistence in the channel of two or more particles is low.

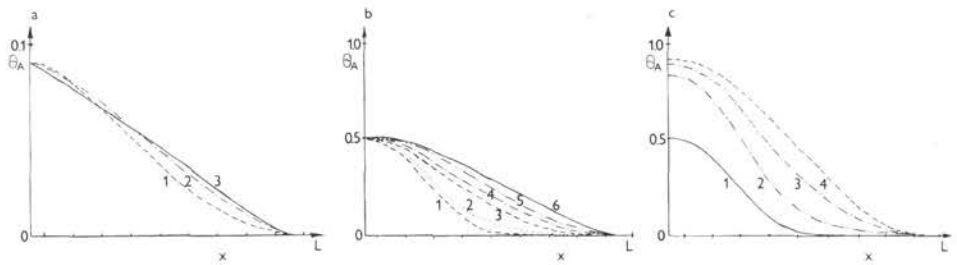


Fig. 8. Profiles of population θ_A: (*a*): (1) $\theta_B(L) = 0.3333$, (2) $\theta_B(L) = 1.667$, (3) $\theta_B(L) = 0.0909$; $\theta_A(1) = 0.0909$ for all curves. (*b*): (1) $\theta_B(L) = 0.9091$, (2) $\theta_B(L) = 0.8333$, (3) $\theta_B(L) = 0.7095$, (4) $\theta_B(L) = 0.6$, (5) $\theta_B(L) = 0.5$, (6) $\theta_B(L) = 0.3333$; $\theta_A(1) = 0.5$ for all the curves. (*c*): (1) $\theta_A(1) = 0.5$, (2) $\theta_A(1) = 0.8333$, (3) $\theta_A(1) = 0.8889$, (4) $\theta_A(1) = 0.9091$; $\theta_B(L) = 0.9091$ for all the curves.

Fig. 8*B* shows that at moderate concentrations, upon an increase in the concentration of one of the solutions, the population profile seems to be "shifted" towards lower concentrations. A similar picture is also obtained at high concentrations (Fig. 8*C*). In addition, the linearity of the population profile for the internal wells of the channel at high and symmetrical concentrations should be stressed, this evidently being due to the "flattening-out" of the corresponding profile $F(AB)$ (Fig. 8*C*).

The qualitative characteristics of the single-file transport process are most pronounced in the profiles of the paired correlation function $F(AB)$. The relations of these profiles to concentrations (or the population of boundary wells), as shown in Fig. 9, are very interesting and have a complex nature. Fig. 9 illustrates these relations with the concentration of one of the solutions being set constant. Consequently, for a low population at equal concentrations (Fig. 9*A*) the profile $F(AB)$ is smoothly sloping, and upon raising one of them the profile is slightly shifted and becomes much higher. The superposition approximation of the paired correlation function $F(AB)$ at such concentrations does not fit well. For moderate concentrations (Fig. 9*B*) a set of bell-shaped curves was obtained with a pronounced envelope. The values of the paired correlation function $F(AB)$ are very close to those obtained in the superposition approximation; the superposition

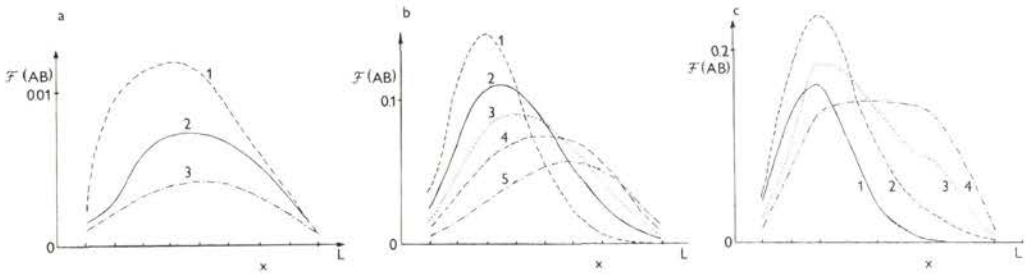


Fig. 9. Profiles of the pair correlation functions $F(AB)$: (*a*): (1) $\theta_B(L)=0.3333$, (2) $\theta_B(L)=0.1667$, (3) $\theta_B(L)=0.0909$; $\theta_A(1)=0.0909$ for all curves. (*b*): (1) $\theta_B(L)=0.8333$, (2) $\theta_B(L)=0.7059$, (3) $\theta_B(L)=0.6$, (4) $\theta_B(L)=0.5$, (5) $\theta_B(L)=0.3333$; $\theta_A(1)=0.5$ for all the curves. (*c*): (1) $\theta_A(1)=0.5$, (2) $\theta_A(1)=0.8333$, (3) $\theta_A(1)=0.8889$, (4) $\theta_A(1)=0.9091$; $\theta_B(L)=0.9091$ for all the curves.

Table 1. Experimentally obtained correlators and functions of them for two specific cases. The number of wells within the channel is 10.

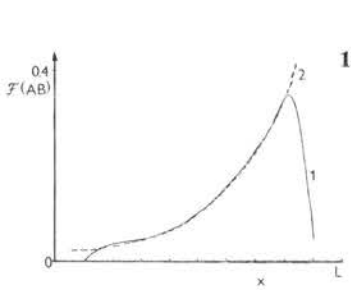
A. $\theta_A(1)=\theta_B(L)=0.231$

Well No	1	2	3	4	5	6	7	8	9	10
Function										
θ_A	0.231	0.215	0.193	0.164	0.133	0.099	0.067	0.037	0.016	0
θ_B	0	0.015	0.038	0.064	0.095	0.129	0.162	0.193	0.215	0.231
$F(AB)$	0.0036	0.0105	0.0154	0.0204	0.0228	0.0210	0.0174	0.0104	0.0038	
$\theta_A(n)\,.\,\theta_B(n+1)$	0.0036	0.0081	0.0124	0.0156	0.0172	0.0160	0.0130	0.0080	0.0038	
$\theta_B(n)\,.\,\theta_A(n+1)$	0	0.0030	0.0062	0.0085	0.0094	0.0085	0.0062	0.0031	0	

B. $\theta_A(1)=0.5$; $\theta_B(L)=0.8333$

Well No	1	2	3	4	5	6	7	8	9	10
Function										
θ_A	0.5	0.462	0.349	0.202	0.091	0.033	0.009	0.0024	0.0005	0
θ_B	0	0.076	0.229	0.414	0.562	0.655	0.715	0.756	0.797	0.833
$F(AB)$	0.0381	0.1141	0.1471	0.1116	0.0572	0.0236	0.0061	0.0018	0.0004	
$\theta_A(n)\,.\,\theta_B(n+1)$	0.0381	0.1060	0.1446	0.1134	0.0599	0.0236	0.0068	0.0019	0.0004	
$\theta_B(n)\,.\,\theta_A(n+1)$	0	0.0266	0.0462	0.0378	0.0186	0.0059	0.0017	0.0004	0	

approximation is the more accurate the steeper the population profile (Table 1). In the symmetrical case, at high concentrations a decrease in one of the concentrations results in the plateau first inclining and then assuming a bell shape; finally, the bell "is lowered" which is evidently associated with an abrupt decrease in the probability for particles of type B to be present in the channel (Fig. 9C).



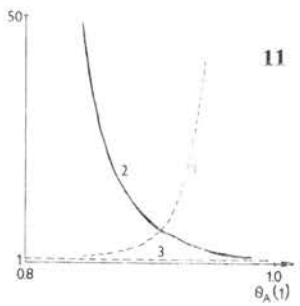


Fig. 10. Profile of the correlation function $F(AB)$ for superhigh concentrations ($\theta_A(1)=0.999$, $\theta_B(L)=0.9985$): (1) $F(AB)$, (2) $(C_A/C_B)^*$ (asterisk denotes the well number).

Fig. 11. Relationship between the length of stacks A and B and the population θ_A of the left boundary well at a fixed population θ_B of the right boundary well ($\theta_B(L)=0.9091$): The length of the stack A (1) and B (2); (3) asymptote.

In the asymmetrical case at high concentrations the inclined plateau for the profile $F(AB)$ represents a masked exponential dependence which becomes pronounced at superhigh concentrations (Fig. 10).

A new and somewhat unexpected result is the observation that particles of the same type leave the channel in "stacks". This implies the following. We shall follow only those events associated with the passing of the particles A through the channel and going into the solution B, or particles B passing through the channel and going into the solution A. Suppose that at a given moment a particle B has passed through the channel subsequently. This passage will be called the start of the stack "A". The number of particles A, which have passed through the channel since this point until the passage of the first particle B, will be called the length of the stack. The relationship between the length of stacks and the population in the boundary wells is shown in Fig. 11.

It is obvious that even at slight deviations from the equilibrium ($C_A \approx C_B$) the stacks length starts increasing drastically. At equal concentrations the stacks have a length not exceeding that of the channel, and upon a slight disbalance of the system they can increase tens of times (in this case the length of the stack of another type — i.e. particles passing in the opposite direction — tends to unity). In case of a considerable disbalance the stacks get so long that they even cannot be computer simulated. This relationship becomes very steep at high concentrations and even steeper with the increasing number of wells within the channel.

Discussion

The computer simulation method enables to obtain both the stationary and dynamic and fluctuation characteristics of the process (e.g. stacks). Hence it has an advantage over the existing analytical methods.

The results of computer simulation have shown that single-filed diffusion is qualitatively different from the ordinary one. For example, the population profiles θ_A and θ_B have nonlinear shapes (Figs. 4, 8) in contrast to the classical case of ordinary diffusion. The relationship between unidirectional fluxes and the corresponding concentrations in the solutions is of interest. For example, particles with a much higher concentration in the solution (e.g. $C_A > C_B$) suppress the counterflux of particles of the other type, transported from the opposite end of the channel (particles B), and their flux through the channel (j_A) approaches to the total flux (j_A). In this case, the flux of particles of the other type (j_B) is exponentially small. Consequently, there is a close relationship between unidirectional fluxes and concentration (or the population of the boundary well) (Fig. 7).

Blocking of particles A by particles B and vice versa plays an important role in single-file diffusion. The probability of a block at some point of the channel is exactly the value of the paired correlation function $F(AB)$ at this point. The profiles of the pair correlation function $F(AB)$ at high concentrations are plateau-shaped. As already mentioned, this is due to the fact that the transport is mediated by scarcely interacting holes. Under these conditions the channel has a small number of degrees of freedom since there are few possible transitions at each moment. On the contrary, at moderate concentrations the channel has many degrees of freedom and this seems to give the profiles of the pair correlation function $F(AB)$ a bell-shape. The point is that, when the system has many degrees of freedom, there are no long-range correlations between the positions of particles within the channel (in contrast to the case of high concentration when all the particles move in the same manner). The absence of long-range correlations allows to speak about a local equilibrium for each well within the channel; consequently, the superposition approximation of the pair correlation function $F(AB)$ becomes valid and the pair correlation function assumes a bell-shaped profile. It is seen from a comparison of the results of computer simulation with those of analytical calculations (Aityan 1985) that the assumption concerning the superposition approximation $F(AB) = \theta_A \theta_B$ (Aityan 1985), works well in the region of moderate populations. In the region of low ($\theta < 1/L$) and high ($1 - \theta < 1/L$) populations the pair correlation function $F(AB)$ is not divided into the product $\theta_A \theta_B$ (the superposition approximation) (Figs. 4, 10). However, at a low population θ the inaccuracy of the approximation $F(AB)$ does not affect unidirectional fluxes because $F(AB) \sim \theta^2$ is of the second order of magnitude in θ as compared with the first order in the diffusion term (Aityan 1985). Thus, the superposition approxima-

tion $F(AB)=\theta_A\theta_B$ gives correct results for unidirectional fluxes at low and moderate populations of the channel. However, the pair correlation functions $F(AB)$ (see Fig. 4) at low and high populations cannot be described in the superposition approximation.

We would like to stress the presence of stacks, revealed by computer simulation, and their strong dependence on small deviations from the symmetry of the system (Fig. 11). This dependence can be accounted for by the fact that even with a slight disbalance of the symmetry of the system a total stationary flux of particles appears, which sharply elongates the stacks of particles transported in the direction of the flux and shortens the stacks of particles transported in direction opposite to the flux. The increase in the stack length with increasing length of the channel and with increasing population seems to be due to the fact that, under these conditions, the correlation length within the channel increases as well.

Computer simulation has thus enabled to disclose the true characteristics of single-file transport and a comparison with the available analytical calculations (Aityan 1985) has made it possible to find the limits of applicability of the assumption made in the paper by Aityan (1984) concerning the superposition approximation of the pair correlation function $F(AB)=\theta_A\theta_B$. Data obtained from computer simulation provide a deeper insight into the physics of the phenomenon investigated and have supplied a good basis for a further comprehensive analysis of the process of single-file transport.

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