Materials Science-Poland, Vol. 24, No. 2/2, 2006

Non-mononotonical behaviour of reaction diffusion front width. Simulation studies in frame of dynamic lattice liquid (DLL) model

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Investigations of anomalous behaviour of the reaction diffusion front for A + B → 2C (inert) and A + B → CC processes are presented. Computer simulation studies were performed using the model of dynamic lattice liquid (DLL) for both two- and three-dimensional cases. Special attention was paid to situations when the mobility of products C and CC significantly differs from the mobilities of reactants. Under such conditions, new kinds of dynamical behaviour were detected. The results obtained indicate that it is necessary to re-formulate the classical description of reaction diffusion front problem. The generalized formalism suggested in the paper should allow a proper description of dynamics of the reaction front over the whole time range including the case when the mobilities of reactants and products are different.

1. Introduction

Reactions at phase boundaries play an important role in many industrial as well as biological processes. The main problem of such reactions is knowledge about formation of so called reaction front between initially separated reactants [1-5]. This phenomenon usually controls the reaction kinetics and can be explained in the following simple way: Initially, two kinds of species (let us denote them A and B) are separated by an impenetrable barrier. The barrier is removed at time $t = 0$ and the reactants start to form a reaction front. The reactant species mix before they react if their mobility is high enough in comparison with their reactivity. This leads to a series of various kinetic regimes between the initial and an asymptotic long time behaviour. To describe an irreversible reaction diffusion process (A + B → 2C, where C is an inert product)

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the following mean-field type equations for the concentration profiles $\rho_A(x,t)$ and $\rho_B(x,t)$ have been used [6]:

$$\frac{\partial \rho_A}{\partial t} = D_A \frac{\partial^2 \rho_A}{\partial x^2} - k\rho_A\rho_B \tag{1a}$$

$$\frac{\partial \rho_B}{\partial t} = D_B \frac{\partial^2 \rho_B}{\partial x^2} - k\rho_A\rho_B \tag{1b}$$

where D_A and D_B are diffusion constants, and k is the microscopic reaction rate constant. These equations must satisfy the initial separation condition along the separation axis x:

$$\begin{aligned} \rho_A(x,0) &= a_0 H(x) \\ \rho_B(x,0) &= b_0\left[1 - H(x)\right] \end{aligned} \tag{1c}$$

where a_0 and b_0 are initial concentrations and $H(x)$ is the Heaviside step function. The problem formulated in Eqs. (1) was investigated using various methods: scaling theory [6–14], experiment [15–17], dimensional analysis [18–20], perturbation theory [21–24], renormalization group technique [25], computer simulation and numerical computation [26–33]. It is necessary to stress that the above description assumes the diffusion as a sole transport mechanism and strictly constant values of the diffusion coefficients of all species (independently of spatial location and concentrations of reactants and products). It means that correlation of movement between A, B (reactants) and C (product) species is neglected. Such treatment seems to be appropriate only in three cases: if the considered time range is short enough (compared to the inverse of the reaction rate) (i), if concentrations of species A and B are low enough (i.e. a correlation between movements of reactants and product species is very weak) (ii) and when the mobilities of all particles are the same (iii). These conditions, however, are satisfied only in some exceptional systems. In general, the mobilities of components are different and the correlation between their movements cannot be neglected, especially for high concentrations of A and B species. A correlation between motions of the species results in a variation of the diffusion coefficients within the reaction zone leading to the kinetic behaviour out of range of the applicability of Eqs. (1). This means that in order to consider more general cases the problem has to be reformulated.

In order to take into consideration a correlation between the movements of A, B and C species and the presence of an inert solvent M, the formula (1) should be extended to the following form:

$$\frac{\partial \rho_A}{\partial t} = \frac{\partial}{\partial x}\left(D_A(x,t)\frac{\partial \rho_A}{\partial x}\right) - k\rho_A(x,t)\rho_B(x,t) \tag{2a}$$

$$\frac{\partial \rho_B}{\partial t} = \frac{\partial}{\partial x}\left(D_B\left(x,t\right)\frac{\partial \rho_B}{dx} \right) - k\rho_A\left(x,t\right)\rho_B\left(x,t\right) \tag{2b}$$

$$\frac{\partial \rho_C}{\partial t} = \frac{\partial}{\partial x}\left(D_C\left(x,t\right)\frac{\partial \rho_C}{dx} \right) - k\rho_A\left(x,t\right)\rho_B\left(x,t\right) \tag{2c}$$

$$\frac{\partial \rho_M}{\partial t} = \frac{\partial}{\partial x}\left(D_M\left(x,t\right)\frac{\partial \rho_M}{\partial x} \right) \tag{2d}$$

where: $\rho_A(x,t)$, $\rho_B(x,t)$, $\rho_C(x,t)$ are local concentrations of the reactants and the product, respectively, $\rho_M(x,t)$ is the concentration of the inert solvent, and $D_A(x,t)$, $D_B(x,t)$, $D_C(x,t)$, $D_M(x,t)$ are the respective local diffusion coefficients. Obviously, this set of equations is very difficult to solve analytically or by a numerical computation because temporal and positional dependencies of local diffusion coefficients are unknown in general case. Only computer simulation on microscopic level can give proper results in this situation. This kind of methods has been successfully used for investigation of the reaction diffusion front problem (lattice gas [26], cellular automata [27, 29, 31]) providing many interesting and stimulating results.

In this work, computer simulation studies are performed using the dynamic lattice liquid (DLL) model for two particular situations: the well known case when mobilities of all types of system components are the same (in order to verify the propriety of the DDL model) (i) and the case when the mobility of the product is considerably lower than the mobilities of reactants (ii). In both cases $a_0 = b_0$ is assumed.

2. Dynamic lattice liquid (DLL) model and simulation conditions

The DLL model is based on the concept of strictly cooperative motions taking place in a dense system of molecules or particles. In contrast to other models taking into account jumps of molecules into free space, the DLL model allows lattice systems with the density factor $\rho = 1$ (i.e., with all lattice sites occupied) to be taken into consideration. The cooperative rearrangements have the form of closed loops of displacements which allow preservation of system continuity. The model was described in detail elsewhere [34, 35], and the aim of this section is only its brief presentation. The DLL model suits very well conditions required for simulation of the reaction front formation due to both, a good agreement with fundamental dynamical properties of liquids, and a simple way of controlling mobilities of different constituents [36, 37].

The simulation algorithm based on the DLL model uses a lattice structure as a discretized space and beads representing small molecules occupying lattice sites. The assumption of a dense packing of molecules leads to the consideration of a system with all lattice sites occupied. It is also assumed that the system has a small excess volume so that each molecule has enough space to vibrate around its equilibrium position defined by the lattice site. However, the molecules cannot easily move over a larger distance because all neighbouring lattice sites are occupied by similar elements. Nevertheless, the DLL model ensures conditions for molecular translation over distances exceeding the vibrational range (long-range mobility). Each large enough displacement of a molecule from its mean position is considered as an attempt of movement to a neighbouring lattice site. For simplicity, directions of the attempts are assumed only along the lattice coordination lines but are independent and randomly distributed among *q* directions, where *q* is the lattice coordination number. Only those attempts can be successful which coincide in such a way that along a path including more than two molecules, the sum of displacements is equal to zero (condition of continuity). This results in displacements of beads along self-avoiding closed paths as is illustrated in Figure 1 (case 5) for a simple 2D liquid on a triangular lattice. Beads which do not contribute to correlated sequences (circuits) are immobilized. This occurs in cases 1–4 illustrated in Table 1. For an athermal system, all possible rearrangements are performed by shifting beads along the closed loop traces, each bead to a neighbouring lattice site. Thus, the following steps can be distinguished in the elementary period (time unit) of the simulation procedure: random generation of the vector field representing attempts of movement (i), elimination of non-successful attempts (ii) and replacing beads within closed loop paths (iii).

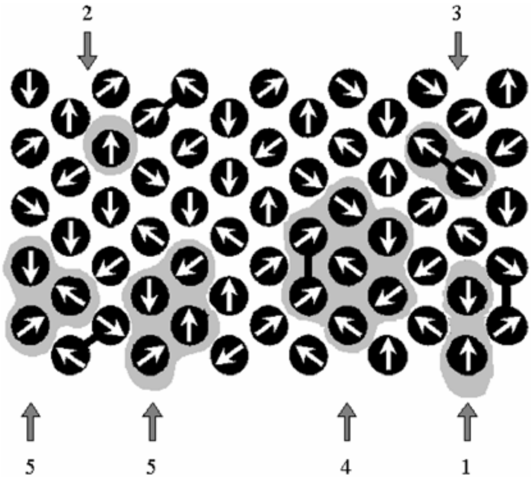
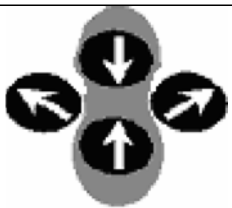
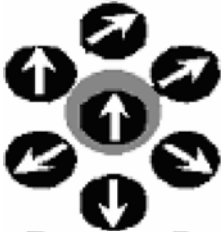


Fig. 1. An illustration of the vector field representing attempts of molecular displacements towards neighbouring sites in the DLL model

Molecular systems treated in this way can be regarded as provided with the dynamics consisting of local vibrations and occasional diffusion steps resulting from coincidence of attempts of neighbouring elements to displace beyond the occupied positions. Within a longer time interval, this kind of dynamics leads to displacements of individual beads along random walk trajectories with steps distributed randomly in time.

Table 1. Special cases of movement towards neighbouring lattice sites

Nr	Variant of movement	Description
1		two neighbouring beads try to move in opposite directions
2		an attempt of motion starts from a lattice site towards which at the same time no other beads are attempting to move
3		attempted movement would lead to a break of a bond in the polymer chain
4		a solvent particle would jump through a bond
5		a cooperative rearrangement along a closed loop

In simulations performed in this study, $N_x \times N_y$ triangular and the $N_x \times N_y \times N_z$ *fcc* lattices were used for two- and three-dimensional cases, respectively. Each model system had been initially divided into two equal parts in which the reactants A and B were distributed with concentrations a_0 and b_0 in such a way as they would be separated by an impenetrable barrier. At time $t = 0$ the barrier was removed and the interdiffusion began allowing AB contacts and the reactions between the species A and B according to one of the two following schemes: A + B = 2C (i) or A + B = CC (ii). In the former case, the reaction resulted in two non-bonded C species, whereas, in the latter case, bonded two bead species were created. The reactions were performed before each DLL motion step according to the following procedure: for each A (B), a neighbouring site was randomly chosen (i); if the chosen site was occupied by B (A), the reaction occurred with an assumed probability p (ii). Mobilities of species C in the first type of reaction were modified with respect to the mobilities of reactants by a reduction of motion probability by a factor Π. The influence of the probability Π on the self-diffusion constant for the triangular and *fcc* lattices was analyzed in our earlier paper [36]. In the second type of reaction, the mobilities of CC species were reduced with respect to mobilities of A and B as a result of the size change. Periodic boundary conditions were applied for the y direction in the two-dimensional case and for the y and z directions in the three-dimensional case. In the x direction, the systems were confined between two neutral impenetrable walls.

In order to characterize the dynamic behaviour of the investigated systems at microscopic and macroscopic levels, the following quantities are considered: local production rate $R(x,t)$, global reaction rate $R(t)$, position of the centre of reaction front $x_f(t)$, width of the front $w(t)$, and height of the front $R(x_f,t)$.

The local production rate of the product C for the A + B → C reaction can be expressed as follows:

$$R(x,t) = k\rho_A(x,t)\rho_B(x,t) \tag{3}$$

This function characterizes the local kinetics but it is a basis for dynamic behaviour of the whole system. The result of a spatial integration over $R(x,t)$

$$R(t) = \sum_x R(x,t) \tag{4}$$

is called global reaction rate $R(t)$ and describes the reaction rate at the macroscopic level.

The position of the centre of reaction front $x_f(t)$ is defined as a position where the $R(x,t)$ function attains maximum

$$\begin{gathered} x_f(t) = x_f(0) + \delta x(t) \\ \delta x_f(t) = \frac{\sum_x \big(x - x_f(0)\big) R(x,t)}{\sum_x R(x,t)} \end{gathered} \tag{5}$$

where $x_f(0)$ represents position of the front at the moment $t = 0$, $\delta x_f(t)$ corresponds to a displacement of the front centre after time t. The width of the front $w(t)$

$$w^2(t) = \frac{\sum_x \big(x - x_f(t)\big)^2 R(x,t)}{\sum_x R(x,t)} \tag{6}$$

and the height of the front (local rate at x_f – $R(x_f,t)$) are the last important quantities describing the diffusion reaction front.

3. Results and discussion

3.1. Reaction fronts in well known cases

In this section, representative results of simulation based on the DLL are presented for the reaction A + B → C under condition of equal mobilities of all particles (i.e., the movement taking place without correlation) and $a_0 = b_0$. This well known case is used here to verify the applicability of the DLL model for description of such a problem. The width of the reaction front $w(t)$, global production rate $R(t)$ and reaction height $R(x_f,t)$ were determined for the system where $\rho_A(x,t) + \rho_B(x,t) + \rho_c(x,t) + \rho_M(x,t) = 1$ (i.e., all lattice sites were occupied by the reactants, the product or the inert solvent), and all elements had a full mobility (i.e. $\Pi = 1$). In a 2D simulation, the triangular lattice was used (size: $N_x = 400$ and $N_y = 400$) while in the 3D case the fcc lattice was employed (size: $N_x = 60$, $N_y = 60$ and $N_z = 60$). The results of each simulation were averaged over 30 trials.

For the case when mobilities of all particles are the same and $a_0 = b_0$, Galfi and Racz [6] found, using scaling arguments, that the width of the reaction front scales with time as $w(t) \propto t^{\alpha}$ with a surprisingly small value of the exponent $\alpha = 1/6$, and the reaction rate at the centre of the front (so called reaction height) scales as $R(x_f,t) \propto t^{-\beta}$ with $\beta = 2/3$. For relatively short times, when a small amount of species react before they become effectively mixed, this system was also studied in the framework of the perturbation theory [30]. A series of crossovers from an initial to an asymptotic time behaviour in the dynamic properties of the reaction front was found. These crossovers depend on the microscopic reaction rate constant k. Basic time dependencies for $w(t)$, $R(t)$ and $R(x_f,t)$ for this case are presented in Table 2.

Table 2. A summary of the cross-over behaviour of the reaction front properties in an initially separated A + B → C reaction-diffusion system

Quantity	Short-time behaviour	Long-time behaviour
$R(t)$	$t^{1/2}$	$t^{-1/2}$
$W(t)$	$t^{1/2}$	$t^{1/6}$
$R(x_f,t)$	const	$t^{-2/3}$

This picture of reaction diffusion front time behaviour was completed by Vilensky et al. [38] who introduced momentum effects which provide to additional early-time regime where the global reaction rate $R(t)$ can increase approximately linearly with time. The results presented in Figures 2 and 3 exhibit a good agreement with the state of the art described above, especially for low values of p (when the influence of fluctuation is low).

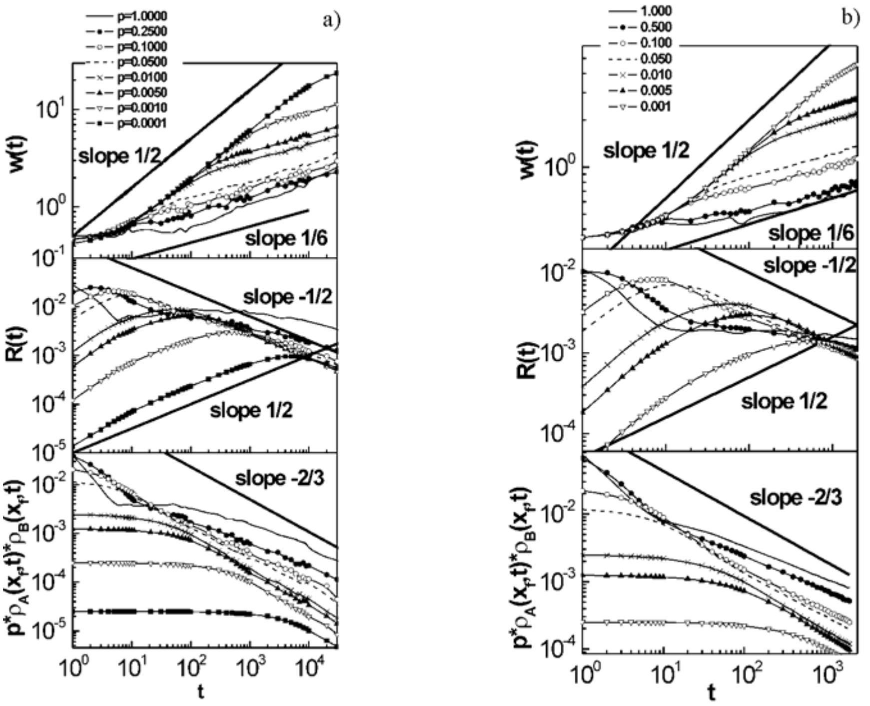


Fig. 2. Time dependencies of $w(t)$, $R(t)$ and $R(x_f,t)$ in the 2D (a) and 3D (b) cases for various probabilities of reaction p. All results were obtained for full mobilities in the system ($\Pi = 1$), and the initial concentration $a_0 = b_0 = 1$

Figures 2a, b show the results obtained for various probabilities of reaction p for the 2D and 3D cases, respectively. In both cases, for high p (i.e., for high reaction rate and influence of fluctuation) characteristic quantities $w(t)$, $R(t)$, $R(x_f,,t)$ deviate from the behaviour predicted by Eqs. (1). At higher ratios of mobility to production rate, however, the agreement of the simulation and theoretical results (calculations based on Eq. (1)) becomes better.

One can see that, in a short time regime for both 2D and 3D cases, $R(t)$ curves increase faster than $t^{1/2}$. This is in agreement with theoretical predictions made by Vilensky et al. [38]. We have to stress that in the 2D case, for small enough probabilities of reaction (i.e., when the species can penetrate each other) we did observe no significant deviation of the $w(t)$ function exponent from the value 1⁄6 in any case. This contradicts the results of Chopard and Droz [29] who reported significant deviation from this value. A decrease of the initial concentrations ($a_0 = b_0$) leads to a displacement of crossovers towards longer due to a lower effective probability of reaction.

Taitelbaum et al. [30] predicted that crossovers depend on the microscopic reaction constant k, and initial concentrations of both reactants. Moreover, changes of $R(t)$ from initial increases to a final decrease take place at time proportional to k^{-1} (in our case, to p^{-1}). Figure 3 presents $w(t)$, $R(t)$, $R(x_f,t)$ for various initial concentrations in 2D case (probability of reaction $p = 0.01$). Figure 4 shows the results representing times corresponding to crossovers for the total production rate $R(t)$ for different initial concentrations (a_0, b_0). One can observe a good agreement of the results obtained by using the DLL model with theoretical predictions.

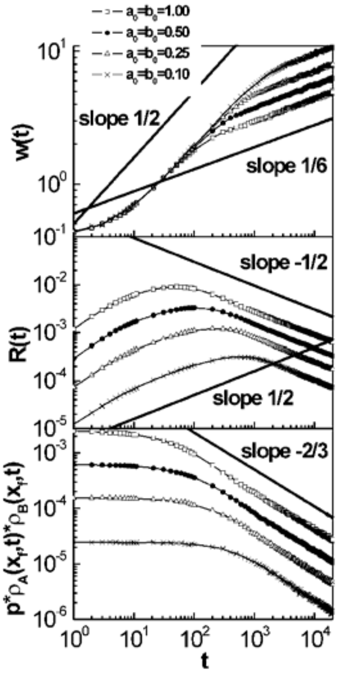


Fig. 3. Time dependencies of $w(t)$, $R(t)$ and $R(x_f,t)$ in the 2D case for various initial concentrations and the same reaction probability $p = 0.01$. All results were obtained for full mobilities in the system ($\Pi = 1$)

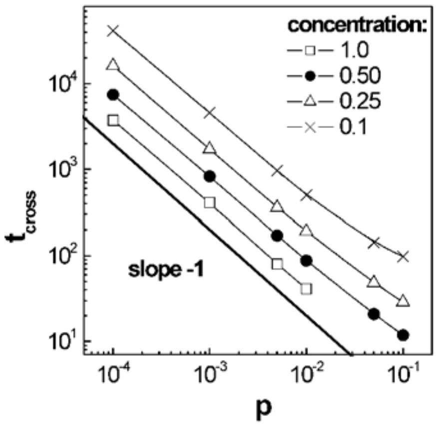


Fig. 4. Position of crossovers for $R(t)$ as a function of p for various initial concentrations

In the situation considered above, one can observe good agreement between the results obtained from the simulation and theoretical predictions when fluctuations can be neglected.

3.2. Role of movement correlation

In this section, we present the results of simulation obtained when the mobilities of reactants and products are different. A decrease of the mobility of products was realized in two ways: by reducing the probability Π of C species (i) and as a result a bond formation between A and B (what is more realistic) when creating the CC species (ii). The results of each series of simulations were averaged over 30 trials.

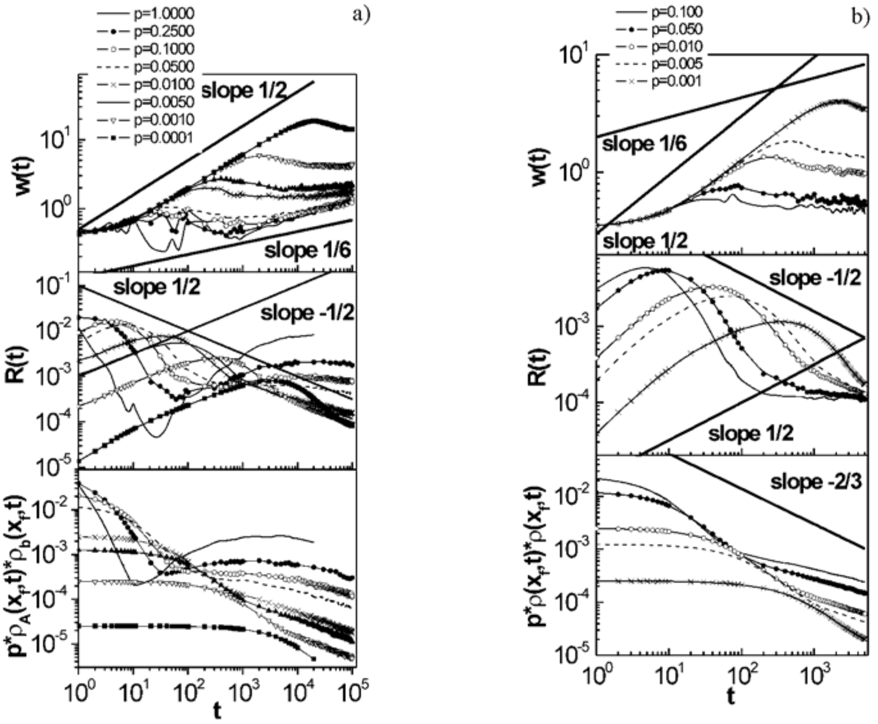


Fig. 5. Time dependencies of $w(t)$, $R(t)$ and $R(x_f,t)$ in the 2D (a) and 3D (b) cases for various probabilities of reaction p. All results were obtained for full mobilities of A and B species ($\Pi = 1$), a reduced mobility of C ($\Pi = 0.25$) and the initial concentration $a_0 = b_0 = 1$

Figures 5a, b (cf. Figs. 2a and 2b) show $w(t)$, $R(t)$ and $R(x_f,t)$ curves obtained by simulations in the 2D and 3D geometries for the situation where the mobility of product C was reduced by taking $\Pi = 0.25$. Figure 6 presents the same time dependencies for the 2D system where the decrease of mobility was realized by the bond formation. In all presented cases, at short times the behaviour of $w(t)$, $R(t)$ and $R(x_f,t)$ does not differ from the results obtained in Section 3 (as was expected). Significant changes can, however, be observed at times longer than the time corresponding to the crossover from the short to long time regime in the case without movement correlation discussed in Section 3. For these times (middle time scale) new crossovers for $R(t)$ and $R(x_f,t)$ curves appear. The reaction rate affects the character and time dependency of these new crossovers, i.e. at higher reaction rates the changes are more dramatic and appear earlier. The behaviour of the width of reaction front *w*(*t*) seems to be particularly interesting: after a time corresponding to short time regime the front becomes narrower.

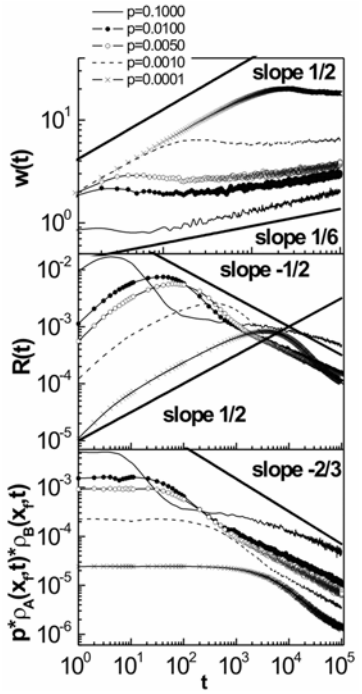


Fig. 6. Time dependencies of *w*(*t*), *R*(*t*) and *R*(x_f,*t*) in the 2D case for various probabilities of reaction *p*. All results were obtained for full mobilities of A and B ($\Pi = 1$), C species connected by bond and the initial concentration $a_0 = b_0 = 1$

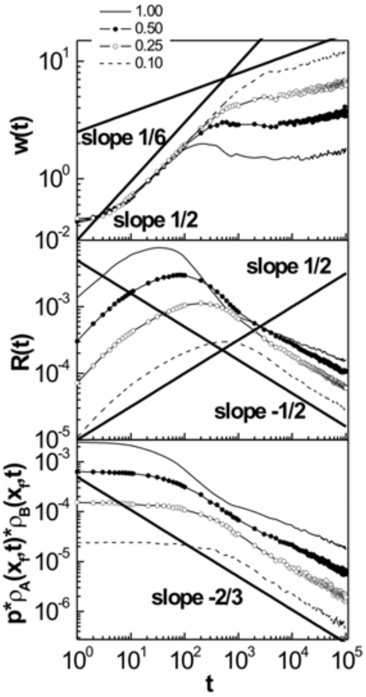


Fig. 7. Time dependencies of *w*(*t*), *R*(*t*) and *R*(x_f,*t*) in the 2D case for various initial concentrations $a_0 = b_0$ and a constant probability of reaction $p = 0.01$. All results were obtained for full mobilities of A and B species ($\Pi = 1$) and a reduced mobility of C ($\Pi = 0.25$)

This behaviour of the reaction diffusion front can be rationalized in the following way: product species formed due to the reaction modify dynamical properties of the reaction diffusion front area making the reactants diffuse slower into this region. This results in a faster decrease of *R*(*t*) and *R*(x_f,*t*) compared to the case without correlation, a decrease of reactant concentration, and hence in a narrowing of the reaction front width. Within the DLL model it means that the probability of the participation of reactant molecules in a cooperative loop decreases as a consequence of the reduced mobility of the product (lower probability of participation of product molecules in cooperative loops) – see also section 2. Additionally, for longer times the slopes of the *R*(*t*) and *R*(x_f,*t*) functions change significantly due to a further mixing (this effect strongly depends on the reaction rate).

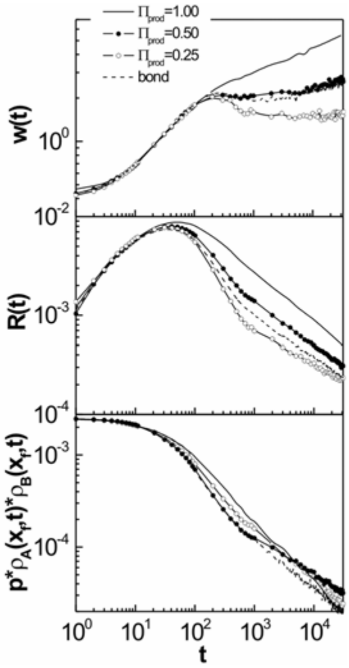


Fig. 8. Time dependencies of $w(t)$, $R(t)$ and $R(x_f,t)$ in the 2D case for various values of Π and a constant probability of reaction $p = 0.01$. All results were obtained for full mobilities of A and B species ($\Pi = 1$) and the initial concentration $a_0 = b_0 = 1$

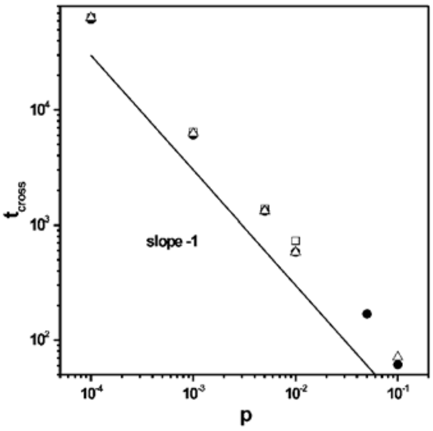


Fig. 9. Position of crossovers in middle time range of $R(t)$ as function of p for the initial concentration $a_0 = b_0 = 1$ and reduced mobilities of C species ($\Pi = 0.25$, $\Pi = 0.50$ and bonded)

Another interesting question is how the effect observed above depends on the initial densities (a_0, b_0) and on the product mobility. Figure 7 shows $w(t)$, $R(t)$ and $R(x_f,t)$ for various initial concentrations (production rate $p = 0.01$). A decrease of the initial concentrations of the reactants leads to a weaker modification of dynamical properties of the reaction diffusion front area. The same behaviour can be observed on lowering the difference between the mobilities of the product and the reactants. Figure 8 presents a comparison between the results obtained for equal or reduced product and reactant mobilities.

Figure 9 shows times corresponding to the crossover discussed above for various Π and the bonded product in 2D. One can infer form the presented results that times at which new crossovers occur are proportional to k^{-1} (in our case, to p^{-1}) similar to changes from short time to long time behaviour in the case without correlation. It is worth to remark that the crossover time is independent of the product mobility for all cases under consideration.

4. Conclusions

The results obtained by simulation based on the DLL model point to a necessity of a reformulation of the description of reaction diffusion front for real systems (systems with different mobilities of reactants and products). In this paper, we propose to replace the commonly used formula (1) by a generalized formula (2) giving a proper picture of the behaviour of the reaction diffusion front over the entire time domain. Taking under consideration dynamical changes of mobility results in this case in a new kinetic behaviour which manifests itself in the appearance of crossovers for the global production rate $R(t)$, reaction height $R(x_f,t)$ and in a non-monotonical behaviour of the width of the reaction front $w(t)$ in the middle time regime. Moreover, the obtained results indicate that it is necessary to adopt a new view on the reaction diffusion front in other systems where observed effects can influence their dynamical behaviour. In particular, this can become important for: non-symmetrical systems ($a_0 \neq b_0$, A and B species have different mobilities) where whole reaction zone can move (i), systems with reversible reactions (ii) and systems with competing reactions (iii). The results presented confirm a large potential of the simulation technique used for getting insight into details of phenomena which are too difficult for analytical theories and which cannot easily be obtained by other simulation methods.

Acknowledgements

The authors would like to thank dr. Z. Koza for helpful discussions. This work was partially supported by KBN (Poland) within the grant projects No. 3 T08A 018 26 and No. 4 T09A 156 2.

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Received 29 April 2005
Revised 30 November 2005