# MOLECULAR DYNAMICS SIMULATIONS OF A PROPAGATING CHEMICAL WAVE FRONT*

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The propagation of a chemical wave front in a nonhomogeneous system with a model reaction $A + B \rightarrow A + A$ is simulated using periodically expanded molecular dynamics technique for reactive hard spheres. It is shown that for fast reactions the speed of a front does not depend on the rate constant as the standard, parabolic reaction-diffusion equation predicts and its value scaled by the square root of the rate constant $k$ is an increasing function of $k$. This phenomenon may be explained on the basis of extended irreversible thermodynamics if separated equations for the concentration of $A$ and for the associated diffusive flow of A are considered.

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## 1. Introduction

The research on spatial- and temporal-selforganization in nonlinear chemical systems, initiated by the discovery of Beolusov–Zhabotynsky reaction in '50s, attracted a lot of scientific attention in the last decade [1].

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Together with the increasing number of experimental results, one can observe a continuous progress in theoretical methods aimed at description of the observed phenomena. The computer simulation methods performed on a microscopic scale (molecular dynamics, lattice gas automata, direct Monte Carlo simulations of Boltzmann equation) play an important role as they allow one to test the theory using model systems, for which all the elementary processes are known.

In this paper we are concerned with molecular dynamics simulations of a chemical wave front propagation. This phenomenon can be regarded as the simplest manifestation of an organized spatio-temporal behaviour in a nonhomogeneous chemical system. Here we consider the simplest chemical wave front which appears in a system with reaction describing quadratic autocatalysis:

$$A + B \xrightarrow{k} A + A. \tag{1}$$

For reaction (1) both states: composed of pure $A$ and composed of pure $B$ are stationary; the first one is stable and the other is unstable. In a nonhomogeneous system a front of concentration of $A$ propagates into regions composed of pure $B$. In our model system described in Chapter 3 the molecules of both $A$ and $B$ are represented by hard spheres characterized by the same mass and diameter and in this particular case it is easy to develop efficient algorithms allowing for simulation at a scale of $10^7$ particles even on a personal computer. Such scale seems to be sufficient for a comparison with the macroscopic theory based on reaction-diffusion equation. Our results show that a standard parabolic reaction-diffusion equation [2] presented in Chapter 2 fails to describe correctly the speed of a front created by a fast reaction. The agreement between theory and simulation can be improved if one uses separated equations for time evolution of concentration and its diffusive flow, as suggested by the extended irreversible thermodynamics [3, 4].

## 2. Equations describing propagation of a wave front

From the assumed reaction scheme (1) it follows that the sum of densities of $A$ and $B$ (denoted as $a$ and $b$ respectively) remains constant ($a + b = n_0$). Therefore the system may be completely described by a single concentration - for example $a$. The "classical" approach to the problem is based on a reaction-diffusion equation, which for reaction (1) has the form [2]:

$$\frac{\partial a}{\partial t} = kab + D\nabla^2 a = ka(n_0 - a) + D\nabla^2 a, \tag{2}$$

where $k$ denotes the rate constant. In simulations we set the reaction rate introducing a steric factor $s_F$ which denotes the probability that a collision

between spheres representing $A$ and $B$ is reactive ($k = s_F k_0$, where $k_0$ is the collision frequency). It is convenient to describe front propagation using the scaled variables: concentration $\alpha = a/n_0$, rate constant $\kappa = n_0 k$ ($\kappa_0 = n_0 k_0$), time $\tau = \kappa t$ and the space variable $\xi = \sqrt{\kappa/D}\mathbf{r}$, where $D$ is the diffusion constant. In these new variables Eq. (2) reads:

$$\frac{\partial \alpha}{\partial \tau} = \alpha(1-\alpha) + \nabla^2 \alpha \,. \tag{3}$$

The studies on equation (3) (and especially on its one dimensional version) have a long history originating from works by Fisher [5] and Kolmogorov *et al.* [6] (for a chronography of research on chemical fronts see [7]). Let us consider a stationary wave front propagating along the $x$-axis with a constant velocity $\nu$. A stationary front profile may be described in the reference frame moving together with it:

$$\alpha(\xi, \tau) = \alpha(\xi_x, \tau) = \alpha(\zeta) \,, \tag{4}$$

where $\zeta = \xi_x - \nu\tau$. The front profile as a function of $\zeta$ variable satisfies equation:

$$\nu \frac{\partial \alpha}{\partial \zeta} + \frac{\partial^2 \alpha}{\partial \zeta^2} + \alpha(1-\alpha) = 0 \,. \tag{5}$$

This equation admits solutions which are stable with respect to local perturbations for all velocities, which are greater or equal than the critical one $\nu_{\min} = 2$ (or in non-scaled variables $v_{\min} = 2\sqrt{\kappa D}$). The particular solution of Eq. (2) which corresponds to $v_{\min}$ is very important because it was shown by Mc Kean [8] that a step-function initial distribution of $A$ evolves into a wave front propagating with this minimal velocity. This result was later generalized by Bramson [9] and by Merkin and Needham [10], who proved that velocity of any front originating from an initial condition, such that the concentration of $A$ vanishes for all $\zeta$ greater than $\zeta_0$, converges to the solution propagating with $v_{\min}$.

Unfortunately, the analytical solution for the profile corresponding to the minimum velocity is not known. An analytical solution, which is quite close to the critical one was given by Kaliappan [11]. It reads:

$$\alpha(\zeta) = \frac{1}{\left(1 + Q \exp\left(\frac{\zeta}{\sqrt{6}}\right)\right)^2} \,,$$

where $Q \geq 0$ is a constant related to the initial condition. The velocity, this solution corresponds to is greater than $v_{\min}$ by a factor $\sqrt{25/24}$.

The shape of fronts profile is uniquely related to the scaled velocity. If one considers the inflection point of $\alpha(\zeta)$ than the following relationship between $\alpha$ and $v$ is hold:

$$v = \nu\sqrt{\kappa D} = -\sqrt{\kappa D}\alpha(1-\alpha)\left(\frac{\partial\alpha}{\partial\zeta}\right)_i^{-1}. \tag{6}$$

An alternative description of a wave front propagation comes from the recently developed methods of extended irreversible thermodynamics [3, 4]. For reaction (1) the coupled equations for the density of $A$ and for the accompanying diffusion flow read:

$$\begin{aligned}\frac{\partial a}{\partial t} &= ka(n_0 - a) - \nabla J_a\,,\\ \frac{\partial J_a}{\partial t} &= -L(J_a + D\nabla a)\,,\end{aligned} \tag{7}$$

where $J_a$ denotes the diffusion flow associated with $a$. Eqs (7) may be considered as describing processes in two different time scales: a slow one for the conserved variable $a$ and a fast one for a non conserved variable $J_a$. If the relaxation of $J_a$ is infinitely fast ($L \to \infty$) then the second equation gives:

$$J_a = -D\nabla a$$

and the set of equations (7) reduces to Eq. (3). Using the same rules of scaling as before, defining the scaled diffusion flow as $\iota_\alpha = J_a/n_0$ and assuming that a front depends only on $\xi$ one obtains:

$$\begin{aligned}\frac{\partial\alpha}{\partial\tau} &= \alpha(1-\alpha) - \frac{\partial}{\partial\xi}\frac{\iota_\alpha}{\sqrt{\kappa D}}\,,\\ \frac{\kappa}{L}\frac{\partial}{\partial\tau}\frac{\iota_\alpha}{\sqrt{\kappa D}} &= -\frac{\partial}{\partial\xi}\alpha - \frac{\iota_\alpha}{\sqrt{\kappa D}}\,.\end{aligned} \tag{8}$$

Finding an analytical equation of this set of equations seems difficult, however an approximation for fronts velocity can be obtained if one assumes that $\kappa/L$ (reaction-diffusion number) is small. In this case we can assume that:

$$\frac{\iota_\alpha}{\sqrt{\kappa D}} \cong -\frac{\partial}{\partial\xi}\alpha + \frac{\kappa}{L}\frac{\partial}{\partial\tau}\frac{\partial}{\partial\xi}\alpha \tag{9}$$

and the equation for wave front is:

$$\frac{\partial\alpha}{\partial\tau} = \alpha(1-\alpha) + \frac{\partial^2}{\partial^2\xi}\alpha - \frac{\kappa}{L}\frac{\partial^3}{\partial\tau\xi^2}\alpha\,. \tag{10}$$

Assuming the stationary form of front solution (Eq. (4)) one obtains the following equation for the profile:

$$\nu\frac{\partial\alpha}{\partial\zeta}+\frac{\partial^2\alpha}{\partial\zeta^2}+\frac{\kappa}{L}\nu\frac{\partial^3\alpha}{\partial\zeta^3}+\alpha(1-\alpha)=0\,. \tag{11}$$

At the inflexion point of the profile one has the following relationship between the derivatives at this point: $(\frac{\partial\alpha}{\partial\zeta})_i$, $(\frac{\partial^3\alpha}{\partial\zeta^3})_i$ and the front's velocity:

$$\begin{aligned} v &= \nu\sqrt{\kappa D} \\ &= -\sqrt{\kappa D}\alpha(1-\alpha)(\frac{\partial\alpha}{\partial\zeta})_i^{-1}\frac{1}{1+\frac{\kappa}{L}(\frac{\partial^3\alpha}{\partial\zeta^3})_i(\frac{\partial\alpha}{\partial\zeta})_i^{-1}}\,. \end{aligned} \tag{12}$$

Let us assume that in the case of small $\kappa/L$ the shape of the front, described in the scaled variables, is the same as the solution obtained for $(\kappa/L)=0$ (and thus it is described by the shape corresponding to the minimum stable velocity). Using Eq. (6) we obtain the following rule of velocity scaling with respect to the steric factor $s_F$:

$$\frac{\sqrt{s_F}}{v}=\frac{1}{2\sqrt{\kappa_0 D}}(1-s_F\gamma)\,, \tag{13}$$

where $\gamma$ denotes $-\frac{\kappa_0}{L}(\frac{\partial^3\alpha}{\partial\zeta^3})_i(\frac{\partial\alpha}{\partial\zeta})_i^{-1}$ and it is easy to show that $\gamma$ is positive.

The assumption on the independence of shape of profile on $s_F$ leads to the conclusion that the value of $\gamma$ is constant for all systems characterized by the same diffusion constant and collision frequency.

Let us notice that the results given by the classical, parabolic reaction diffusion equation and by the extended irreversible thermodynamics are qualitatively different. The first method says that the scaled speed of a front is constant, in the second this speed is an increasing function of $s_F$.

## 3. Molecular dynamics simulations of wave front propagation

Molecular dynamics technique [12] seems to be the most appropriate for microscopic simulations of chemical systems. On the other hand, the method is the most demanding from the computational point of view. Therefore, alternative techniques, like the Bird method [13] or cellular gas automata [14] were used to simulate propagation of a chemical wave front [15]. However, both these techniques involve significant approximations. In the Bird method the system is divided into subcells, within which the collisions are unrelated to the actual positions of particles (it means that

the spheres, which collide are randomly chosen). The lattice gas automaton introduces an artificial lattice geometry of the system and a particle jumps to one of the nearest nodes within a single time step. Therefore the speeds of all particles are the same and the method cannot be applied to thermally activated reactions, in which one may expect significant difference in velocities of particles corresponding to reactant and product [16].

In this paper we apply a new simulation technique (periodically expanded molecular dynamics) [17], which allows to perform large scale simulations without simplifications mentioned above. The simulations are based on the model of reactive hard spheres [18]. According to this model all the particles are represented by identical hard spheres (*i.e.* characterized by the same mass and diameter). The chemical identity parameter which describes the "chemical" properties of a sphere, has no influence on its mechanical motion. A reaction may occur if spheres representing the appropriate reactants collide and after such collision the spheres are marked as products. Within this model the lifetime of a transient complex is zero as the reactants are instantaneously transformed into products. The infinitely short time of chemical reactions at a molecular level is clearly separated from the characteristic time for collective phenomena, which is related to an average time between collisions.

A significant increase in the efficiency of simulations performed for reactive hard spheres can be achieved if the periodic expansion of a simulated system is used. Let us assume that all the collisions (including reactive ones) are elastic from the mechanical point of view. In this case a trajectory, which describes the motion of reagents is just an equilibrium trajectory of spheres. On the other hand a "chemical" evolution may be easily obtained from any equilibrium trajectory if the chemical identity parameter is assigned to all particles and if it is updated after every collision regarded as reactive. A prerecorded trajectory acts as a database containing the information on times of collisions and on particles involved in a considered system. If the periodic boundary conditions have been used to generate the equilibrium trajectory, than the size expansion is possible. The periodic boundary conditions mean that the simulated system is regarded as an elementary cell in an infinite system, which is invariant with respect to the translations by the vectors of the side length. The most popular shape of simulated area are: square in the case of a 2D system and a cube in 3D. Knowing the evolution within a single cell one has the information about positions and velocities for corresponding (by symmetry) particles in all its replicas. Therefore, using a prerecorded data on the sequence of occurring collisions one can obtain the evolution of a system which is extended by a number of cells in each direction. Of course, the original periodic boundary conditions remain satisfied for the extended system.

If a chemical identity of molecules is neglected than such expansion does not bring us any new information, as the evolution in all cells of the extended system is identical. Moreover, it may lead to wrong conclusions as the correlations extending over a single cell are affected by artificially introduced periodicity. However, for a multicomponent chemical system, in which the translational motion is not related to chemical identity, the situation is different. First, a different chemical composition may be initialized in various cells by marking the equivalent (by periodicity) spheres in a different way. Secondly, a steric factor if it is not equal to unity, differentiate the "chemical" evolution, because a collision between the same objects may be reactive in one cell and nonreactive in another. Thanks to the periodic boundary conditions a free flow of molecules, between the neighboring cells is ensured. Therefore, one obtains the evolution of a system which is much larger than the original one.

Of course, the simplifications involved introduce unrealistic constrains in the simulated system treated as a whole. The momentum of all particles within each single replica of the original cell is equal to zero, whereas one might expect that this condition should be satisfied for the whole system only. Moreover, the fluctuations of velocity are related to the size of the original simulation cell. It can be expected that the appearance of a particle characterized by a very high velocity is less probable in simulations performed using periodically expanded molecular dynamics than in a system of the same size simulated with the use of the direct method. We believe that both these disadvantages are not important if the number of particles in the original cell is sufficiently large and if the processes considered do not require molecules with a very high energy.

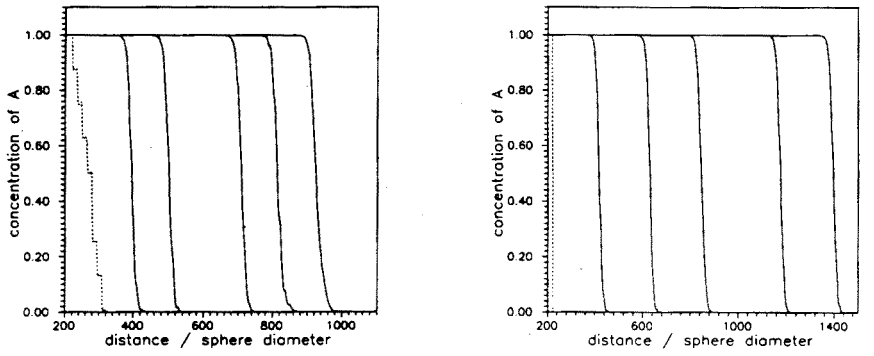
The main advantage of the periodically expanded molecular dynamics is the fact that the method is extremely efficient from the computer point of view. In the case of chemically reacting hard spheres only times and identities of colliding spheres have to be recorded in order to restore a trajectory. To describe an expanded system one needs only one large array in the computer memory to store the actual chemical identities of all objects, whereas all the other quantities as velocities, positions and moments of collisions are periodic in space and they do not require a large memory. A single collision data obtained from a prerecorded trajectory give us information on a set of collisions occurring in all the replicas of the original cell. Therefore, the space required to record a long trajectory is much reduced if compared with the system of the same number of molecules in which the collisions in different regions of space are uncorrected. The scale of simulations (number of collisions per particle) is the same in the expanded system as in the original one.

The results of our simulations were obtained by a periodic expansion of a few equilibrium trajectories, which were recorded for a system composed of hard spheres characterized by the mass $m = 32$ a.u. and diameter the $\sigma = 5$ Å. The average kinetic energy of spheres corresponded to temperature 300 K, but this value is not very important, as temperature may be easily changed by rescaling time. Two different densities were considered. The original simulations at a low density were done for $N = 500$ spheres placed in a cubic box with the side length $d = 14.7\sigma$ and thus the packing fraction was $\eta = 0.0824$. In order to see which is the statistical error of the method, we considered two independent trajectories, each 400000 collisions long. The simulations for a high density system involved $N = 1000$ spheres moving in a cube with the side length $d = 15.5\sigma$ and the packing fraction was $\eta = 0.1406$. This trajectory was over 600000 collisions long.

The system was initialized as homogeneous in $x$ and $y$ directions, which means that the initial average concentrations of $A$ and $B$ in all the cells characterized by the same range of the $z$-variable were the same. For an expanded system the periodic boundary conditions were used in $x$ and $y$ directions. In order to observe front propagation the initial concentration of reactants were nonhomogeneous in the $z$ direction. Part of the simulations started form an initial concentrations described by a step-function: all the spheres, for which $z \leq z_0$ were marked as $A$, all the other as $B$. In other simulations there was a wide interval of $z$ (usually about $100\sigma$ in length) within which the initial concentrations of both reactants were different from zero. A modified periodic boundary conditions (the chemical identity parameter of a sphere crossing the boundary of an expanded system was reversed) were used in the $z$ direction. To analyze the results, the system was divided into slices perpendicular to the $z$-axis (500 total). The fraction of particles representing each of reactants is averaged within every slice.

Most of the simulations for the low density were performed for a system expanded by 14 side lengths in $x$ and in $y$ directions and by 100 side lengths in the $z$ direction. Thus, the total number of spheres considered was 9,800,000. A few simulations were done for a smaller system (expanded 10 times in $x$ and $y$ directions) in order to check if the scale of expansion affects the results.

Fig. 1. shows the time evolution of fronts of concentration which were initiated by a wide (Fig. 1A) and a sharp (Fig. 1B) profile of $A$. The steric factor is $s_F = 0.22$, which means that 22% of collisions between $A$ and $B$ are reactive. As Fig. 1 shows, a well developed, stationary concentration profile appears within less than 100 ps. Observing the distance travelled by a front as a function of time it is easy to obtain the phase velocity as a function of the rate constant (in practice we focused our attention on the shift of a point




(A) (B)

Fig. 1. The profile of concentration of $A$ for a few selected moments of time for a system characterized by the low density and $s_F = 0.223$. The dashed line shows the initial concentration of $A$. The solid lines from left to right correspond to times:
(A) 104 ps, 208 ps, 416 ps, 519 ps and 622 ps;
(B) 208 ps, 416 ps, 622 ps, 934 ps and 1140 ps.

corresponding to $\alpha = 0.5$). For simulations performed at the same packing fraction, the diffusion constant does not change. For the low density, by substituting the values of the diffusion constant ($D = 0.62\ \sigma^2/\text{ps}$) and of the collision frequency ($\kappa_0 = 0.766\ \frac{1}{\text{ps}}$), to the expression for the minimum stable velocity one obtains that:

$$\frac{v}{\sqrt{s_F}} = 2\sqrt{\kappa_0 D} = 1.378\ \frac{\sigma}{\text{ps}}$$

or

$$\frac{\sqrt{s_F}}{v} = 0.726\ \frac{\text{ps}}{\sigma}.$$

The results are shown in Table I. For the slowest reaction the minimum stable velocity is a good approximation of the observed speed of a front. However, the velocity scaled by a square root of the steric factor is an increasing function of $s_F$. This effect cannot be explained on the basis of a standard parabolic reaction-diffusion equation (2).

On the other hand we can adjust the modified expression for velocity (Eq. (13)) to the results of simulations. If one uses the value of $2\sqrt{\kappa_0 D}$ given above then for $\gamma = 1.066$ a good approximation for the observed velocities is observed. The comparison between theory and simulations is presented in Table I. and in Fig. 3A.

TABLE I

The speed of a wave front in ($\sigma$/ps) units; comparison of simulation data with the theory. The packing density is equal to $\eta = 0.0826$. According to the standard reaction-diffusion equation (Eq. (2)) the value of $v/\sqrt{s_F}$ does not depend on $s_F$ and is equal to 1.378 (or $(\sqrt{s_F}/v) = 0.726$ ps/$\sigma$).

| $s_F$ | $\frac{v}{\sqrt{s_F}}$ – simulations | $\frac{\sqrt{s_F}}{v}$ – simulations | $\frac{\sqrt{s_F}}{v}$ – Eq. (13) |
|---|---|---|---|
| 0.02[a] | 1.353 | 0.739 | 0.7044 |
| 0.05[a] | 1.516 | 0.660 | 0.672 |
| 0.1[a] | 1.719 | 0.581 | 0.619 |
| 0.1[b] | 1.723 | 0.580 | 0.619 |
| 0.135[a] | 1.861 | 0.535 | 0.582 |
| 0.135[b] | 1.876 | 0.533 | 0.582 |
| 0.223[a] | 2.157 | 0.457 | 0.488 |
| 0.223[b] | 2.224 | 0.450 | 0.488 |
| 0.368[a] | 2.617 | 0.380 | 0.334 |
| 0.368[b] | 2.655 | 0.377 | 0.334 |

[a] Runs starting from the sharp initial distribution of concentration.

[b] Runs starting from a wide (about 100 $\sigma$) distribution of concentrations.

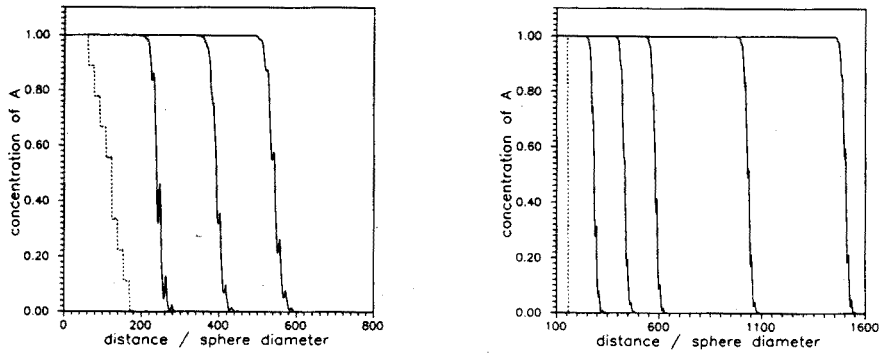
For the system characterized by the high density most of simulations were performed for a system expanded by 10 side lengths in $x$ and in $y$ directions and by 120 side lengths in the $z$ direction. The total number of spheres considered was 12,000,000. For small steric factors we simulated a system, expanded by 14 side lengths along $x$ and $y$ directions and by 70 side lengths in $z$ direction (13,720,000 spheres total). Fig. 2. shows a typical evolution of concentration of $A$ in the high density system. In this case steric factor is $s_F = 0.20$. For the high density ($D = 0.35\frac{\sigma^2}{\text{ps}}$) and ($\kappa_0 = 1.56\frac{1}{\text{ps}}$), so the scaled minimum stable velocity equals:

$$\frac{v}{\sqrt{s_F}} = 2\sqrt{\kappa_0 D} = 1.484\,\frac{\sigma}{\text{ps}},$$

or

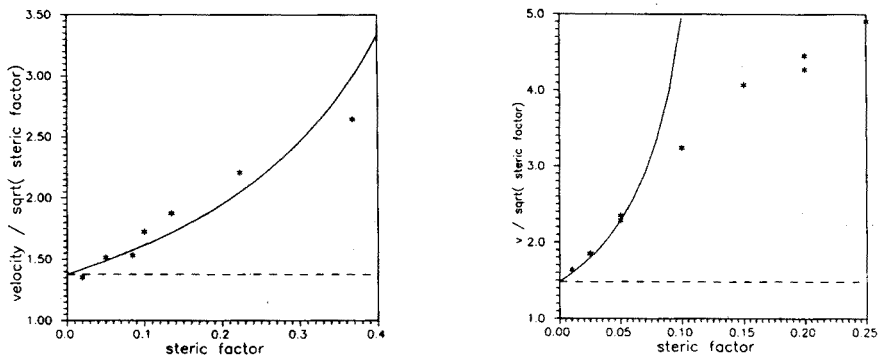
$$\frac{\sqrt{s_F}}{v} = 0.674\,\frac{\text{ps}}{\sigma}.$$

These values agree with the velocities of fronts created by slow reactions ($s_F \leq 0.025$) (see Table II). Simulations performed at the high density also show that the velocity is an increasing function of a steric factor. The change in velocity with respect to $v_{\min}$ corresponding to a given value of $s_F$ is much larger than it was for the low density, as illustrated in Fig. 3B. A simple numerical fit of velocities observed for small steric factors gives $\gamma = 7$, however the linear approximation (Eq. (13)) fails for $s_F > 0.1$.




(A) (B)

Fig. 2. The profile of concentration of $A$ for a few selected moments of time for a system characterized by the high density and $s_F = 0.2$. The dashed line shows the initial concentration of $A$. The solid lines from left to right correspond to times:
(A) 77 ps, 154 ps and 231 ps;
(B) 77 ps, 154 ps, 231 ps, 461 ps and 692 ps.




(A) (B)

Fig. 3. The front velocity scaled by $\sqrt{s_F}$ as a function of steric factor; stars mark the results of simulations, dashed line shows the minimum stable velocity and the solid line is a numerical fit based on Eq. (13).
(A) low density system ($\gamma = 1.066$);
(B) high density system ($\gamma = 7.0$).

TABLE II

The speed of a wave front in ($\sigma$/ps) units for a reaction without thermal activation; comparison of simulation data with the theory. The packing density is equal to $\eta = 0.1406$. According to the standard reaction-diffusion equation (Eq. (2)) the value of $\frac{v}{\sqrt{s_F}}$ is equal to 1.484 (or $\frac{\sqrt{s_F}}{v} = 0.674$ ps/$\sigma$).

| $s_F$ | $\frac{v}{\sqrt{s_F}}$ - simulations | $\frac{\sqrt{s_F}}{v}$ - simulations | $\frac{\sqrt{s_F}}{v}$ - Eq. (13) |
|---|---|---|---|
| 0.01[a] | 1.640 | 0.610 | 0.627 |
| 0.025[b] | 1.855 | 0.554 | 0.556 |
| 0.025[a] | 1.847 | 0.541 | 0.556 |
| 0.05[b] | 2.285 | 0.438 | 0.438 |
| 0.05[a] | 2.350 | 0.426 | 0.438 |
| 0.1[b] | 3.241 | 0.306 | 0.202 |
| 0.15[b] | 4.075 | 0.245 | – |
| 0.20[b] | 4.280 | 0.234 | – |
| 0.20[a] | 4.460 | 0.224 | – |
| 0.25[a] | 4.908 | 0.203 | – |

[a] Runs starting from the sharp initial distribution of concentration.

[b] Runs starting from a wide (about 100 $\sigma$) distribution of concentrations.

## 4. Conclusions

Periodically expanded molecular dynamics technique allowed us to perform a large scale computer simulations on propagation of chemical fronts. The results seems to be accurate enough to measure the speed of a front and to show that in the case of very fast reactions (large reaction-difussion number) the velocity scaled by the square root of the steric factor is an increasing function of $s_F$. Therefore, the standard approach based on a parabolic reaction-diffusion equation (Eq. (2)) fails.

We explained the increase in scaled front velocity using coupled equations for the concentration of reactant and for its diffusive flow (Eqs (7)), as suggested by the extended irreversible thermodynamics. Introducing a few approximations, which seem to be justified for small values of the reaction-diffusion number, we derived a simplified formula for front's velocity (Eq. (13)), which predicts that it is inversely proportional to $(1 - \gamma s_F)$, where $\gamma$ depends on density only. This approximation gives a fair agreement with results of simulations.

The research on wave front propagation may be regarded as a building block for the theory of more complex selforganization phenomena as

chemical spirals or patterns growth. We believe that the developed numerical algorithms can be applied in future microscopic simulations of their dynamics.

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