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Irreversible A + B → 0 Reaction – Diffusion Process with Initially Separated Reactants: Exponential Temporal Asymptotics

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We study theoretically and numerically the irreversible A + B → 0 reaction-diffusion process of initially separated reactants occupying the regions of lengths L_A, L_B comparable with the diffusion length (L_A, $L_B \sim \sqrt{Dt}$, here D is the diffusion coefficient of the reactants). It is shown that the process can be divided into two stages in time. For $t << L^2/D$ the front characteristics are described by the well-known power law dependencies on time, whereas for $t > L^2/D$ these are well approximated by exponential laws. To confirm the obtained theoretical results, a numerical simulation of the reaction has been carried out. The simulation is based on the Monte-Carlo methods. The results of the numerical simulation are presented in Figs. 1 and 2. The numerical simulation properly confirms the obtained asymptotical temporal dependencies of the reaction front characteristics.

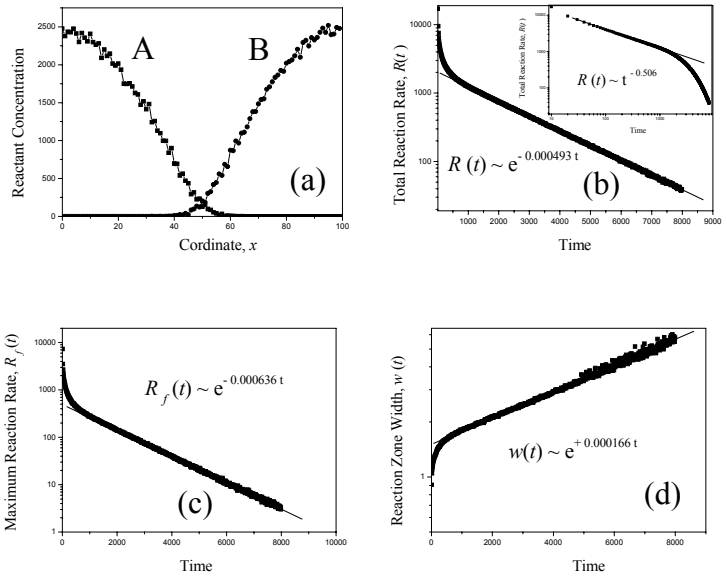

Fig. 1. Numerical simulation of the reaction-diffusion process for the case of equal diffusion coefficients, $D = D_A = D_B = 0.5$ (the probabilities of unit jumps to the left and to the right are 0.5): the distribution of the particle density at $t = 8000$ (a); the temporal dependencies of the total (b) and maximum (c) reaction rates and of the reaction zone width (d). Insert in (b) presents the temporal dependence of the total reaction rate at $t << L^2/D$. Reaction probability is 0.0001, the initial particle concentrations are 100,000. The numerically obtained constants in the exponent indexes agree with the theoretically predicted constant, which for the chosen parameters D and L is 0.000493.

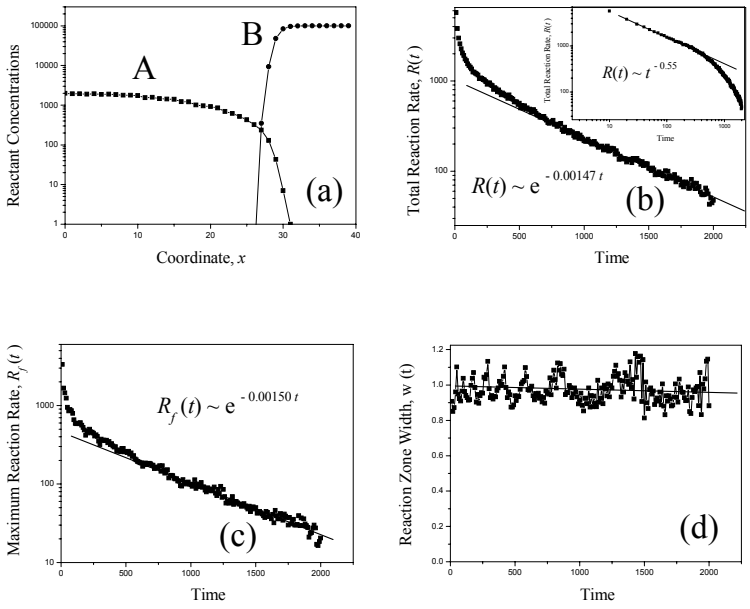

Fig. 2. Numerical simulation of the reaction-diffusion process for the case of immovable B particles. The initial particle concentrations are: $N_{B0} = 100{,}000$, $N_{A0} = 50{,}000$, and $D_B = 0$, $D_A = 0.5$. The distribution of the particle density at $t = 2000$ - (a); the temporal dependencies of the total (b) and maximum (c) reaction rates and of the reaction zone width (d). Insert in (b) presents the temporal dependence of the total reaction rate at $t << L^2/D$. Reaction probability is 0.00001. In the asymptotic time regime L_A is about 29 (see (a)). The numerically obtained constants in the exponent indexes agree with the theoretically predicted constant, which for the chosen parameters D and L_A is 0.00147.