

Reaction front dynamics of $A + B \rightarrow C$ with initially separated reactants

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We study the reaction front for the diffusion–reaction system $A + B \rightarrow C$ with initially separated reactants. We present analytical results for the form of the front and the exponents that characterize its width and height asymptotically, which appear to hold in $d \geq 2$. We also present analytical and numerical results for the form of the reaction front for the 1D case in which one of the reactants is static, and find the width exponent $\alpha = 1/4$, which is larger than the mean field exponent ($\alpha = 1/6$) but smaller than the value for the case in which both species diffuse ($\alpha \approx 0.3$).

Recently there has been considerable interest in the study of the irreversible reaction $A + B \rightarrow C$ (inert) in which the reactants are transported by diffusion and are initially separated in space [1–9]. Under these conditions the system is characterized by a “reaction front” that develops at the interface between the two reactants, and that is marked by the presence of the inert C particles.

The time evolution of the reaction front is usually characterized by two exponents, α and β , that describe how its width ($w \sim t^\alpha$) and height ($h \sim t^{-\beta}$) vary asymptotically with time. Gálfi and Rácz [1], using “mean field” arguments, found scaling relations for these two exponents for the case in which both reactants move, which give the values $\alpha = 1/6$ and $\beta = 2/3$. These exponents have been confirmed experimentally [8] and numerically [2,4, 8]. More recently, the explicit form of the front was obtained analytically [7] as the solution of the mean field reaction–diffusion equations believed to describe the system. It was found that the reaction front $R(x, t)$ had the form (see fig. 1)

$$R(x, t) \sim t^{-2/3} \left(\frac{|x|}{t^{1/6}} \right)^{3/4} \exp \left[-\frac{2}{3} \left(\frac{\lambda|x|}{t^{1/6}} \right)^{3/2} \right]; \quad (1)$$

in the region $t^{1/6}/\lambda < |x| < t^{1/2}/a$, where λ and a are constants that depend on the details of the system. This form, which is consistent with the mean field

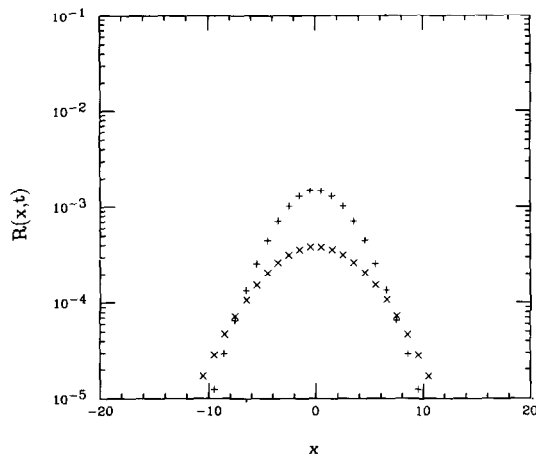


Fig. 1. Reaction front profile $R(x, t)$ near the origin calculated by exact enumeration using the discrete version of the mean field diffusion-reaction equations [7] for $t = 500$ (+) and $t = 1000$ (x).

exponents, and appears to be valid for $d \geq 2$ in agreement with MC simulations of instantaneous reactions [7].

In $d = 1$, numerical data [3,5] indicate that the width and height exponents are $\alpha \approx 0.3$ and $\beta \approx 0.8$, respectively; and up to now there is little understanding of the origin of these values.

In order to gain some insight on the behavior of 1D systems, we consider the case in which only one of the two species move [9]. Specifically, we consider a system in which a particle of species A is initially placed at every site on the left of the origin, and a particle of species B is placed on every site on the right. We only allow the A particles to diffuse. Under these conditions, the initial position of the interface separating both species is at the origin, and moves to the right as $t^{1/2}$. By studying the motion of the leftmost particle of the static reactant B, we find that the reaction front has the form (see fig. 2)

$$R(x, t) \sim t^{-3/4} \exp\left(-\frac{(x - at^{1/2})^2}{bt^{1/2}}\right) \left(1 + \frac{x - at^{1/2}}{2at^{1/2}}\right) \quad (2)$$

and therefore the width and the height are characterized by the exponents $\alpha = 1/4$ and $\beta = 3/4$. In this case the width exponent α has a value intermediate between the case in which both species move and the mean field found by Gálfi and Rácz.

The value $\alpha = 1/4$ should correspond to a lower bound for the case in which both reactants move. This can be understood qualitatively by noting that if

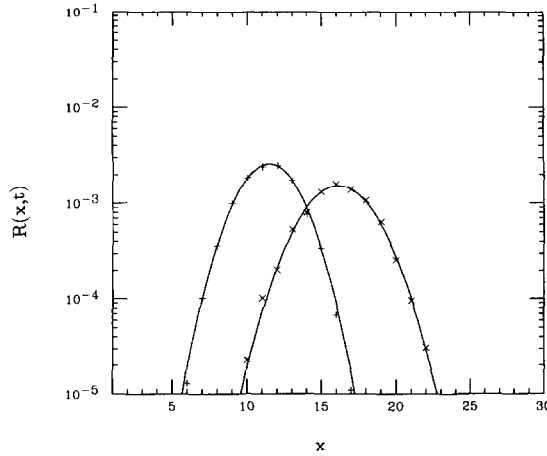


Fig. 2. Reaction front profile $R(x, t)$ calculated from eq. (2) for $t = 500$ and $t = 1000$. The points represent data obtained from Monte Carlo simulations: (+) $t = 500$ and (\times) $t = 1000$.

both reactants move, the boundary between them has the opportunity to “diffuse” in the increasing intervals between reactions.

For higher dimensions ($d \geq 2$), scaling arguments similar to those of Gálfi and Rácz [1] suggest that if only one of the reactants diffuses, then the exponents characterizing the reaction front are $\alpha = 0$ and $\beta = 1/2$ [2], and there may be a logarithmic dependence with time in $d = 2$ [10].

It should be noted that for all the cases mentioned here, the scaling relation $\alpha - \beta = -1/2$ holds [1]. This relation comes from the observation that the reaction rate is $wh \sim t^{-1/2}$. Note that the width of the reaction front always grows slower than the characteristic length of the diffusion process.

The Center for Polymer studies is supported by grants from NSF and ONR. MA acknowledges the support of Intevop S.A. Venezuela, HL the support of CONACYT Mexico while SH thanks the US–Israel Binational Science Foundation for partial support.

References

- [1] L. Gálfi and Z. Rácz, *Phys. Rev. A* 38 (1988) 3151.
- [2] Z. Jiang and C. Ebner, *Phys. Rev. A* 42 (1990) 7483.
- [3] S. Cornell, M. Droz and B. Chopard, *Phys. Rev. A* 44 (1991) 4826.
- [4] H. Taitelbaum, S. Havlin, J. Kiefer, B.L. Trus and G.H. Weiss, *J. Stat. Phys.* 65 (1991) 873; H. Taitelbaum, Y.E. Koo, S. Havlin, R. Kopelman and G.H. Weiss, *Phys. Rev. A* 46 (1992) 2151.

- [5] M. Araujo, S. Havlin, H. Larralde and H.E. Stanley, *Phys. Rev. Lett.* 68 (1992) 1791.
- [6] E. Ben-Naim and S. Redner, *J. Phys. A* 25 (1992) L575.
- [7] H. Larralde, M. Araujo, S. Havlin and H.E. Stanley, *Phys. Rev. A* 46 (1992) 855.
- [8] Y.E. Koo, L. Li and R. Kopelman, *Mol. Cryst. Liq. Cryst.* 183 (1990) 187; Y.E. Koo and R. Kopelman, *J. Stat. Phys.* 65 (1991) 893.
- [9] H. Larralde, M. Araujo, S. Havlin and H.E. Stanley, preprint.
- [10] J. Krug and P. Meakin, *Phys. Rev. Lett.* 66 (1991) 703.