Scaling Effects and Front Propagation in a Class of Reaction-Diffusion Equations: from Classic to Anomalous Diffusion

Andrea Pietro Reverberi[1]*, Agostino Giacinto Bruzzone[2], Bruno Fabiano[3]

1 DCCI – Chemistry and Industrial Chemistry Dept., Genoa University, via Dodecaneso 31, 16146 Genoa (Italy);
2 DIME – Mechanical Engineering, Energy, Logistics and Transports Dept., Genoa University, via Opera Pia 15,
16145 Genoa (Italy); 3 DICCA – Civil, Chemical and Environmental Engineering Dept., Polytechnic School - Genoa
University, via Opera Pia 15, 16145 Genoa (Italy)

*Corresponding author: reverb@dichep.unige.it

Highlights
- A reaction-diffusion equation with non-constant diffusivity and non-linear kinetics is solved.
- The combined effects of such non-linearities on diffusion fronts have been discussed.
- Some new results on the dynamics of diffusion fronts at early times have been shown.
- Numerical results are supported by a newly developed analytical approach.

1. Introduction

When reaction-diffusion processes are investigated according to a mean-field continuum modelling in one spatial dimension for q diffusing/reacting species, a mass balance is combined with a phenomenological equation containing a link between the local flux J and the corresponding driving force as follows:

$$
\begin{cases}
\dfrac{\partial c_i}{\partial t} + \dfrac{\partial J_i}{\partial x} = R_i(\underline{c}) \\[2mm]
J_i(x) = -D_i(\underline{c})\dfrac{\partial c_i}{\partial x}
\end{cases}
\tag{1}
$$

where i is the component index with $1<i<n$, $\underline{c} = (c_1, c_2, \ldots c_n)$ is the concentration vector, x is the space variable, $R(\underline{c})$ is the generation/depletion term and $D(\underline{c})$ is a diffusivity that can be considered as a function of concentrations in case of correlated motion.

Eq.(1) implies different front propagation regimes according to a classical, super- or subdiffusive trend described by:

$$
s(t) = k_1 t^{\alpha} \quad ; \quad \sigma(t) = k_2 t^{\beta}
\tag{2}
$$

where $s(t)$ and $\sigma(t)$ are the average position and the width of the diffusion front of the species c_i, t is the time and k_j are constant prefactors. In case of classical diffusion (Fickian or Fourier, for mass or heat transfer, respectively), $\alpha=\beta=0.5$, while α differs from this value in case of anomalous diffusion.

In the present study, we propose a scalar scheme *(n=1)* where a single diffusing reactant A is depleted along its walk with a diffusivity taking into account attractive and repulsive interactions between moving species.

2. Methods (The Model)

The reaction-diffusion equation and the relevant expressions for diffusivity $D(c)$ and chemical kinetics $R(c)$ here adopted without loss in generality are:

$$
\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}\left(-D(c)\frac{\partial c}{\partial x}\right) = R(c) \; ; \; D(c) = D_0 \exp\left(k\frac{c-c_1}{c_0-c_1}\right) \; ; \; R(c) = -\mu c^{\gamma}
\tag{3}
$$

with $c(0,t)=c_0$ and $c(x,0)=c_1$, $x\neq 0$. It holds that $k>0$ and $D'(c)>0$ for repulsive interactions between diffusing species, while $k<0$ and $D'(c)<0$ for attractive interactions. In the absence of a real physical interface separating different phases typical of moving boundary problems [1], the average position of the moving front can be defined as:

$$s(t) = <x(t)> = \frac{\int_{c_1}^{c_0} x(c)dc}{c_0 - c_1} \tag{4}$$

3. Results and discussion

Two different simulation runs were carried out for $\mu=0$ (null kinetic term) and for $\mu>0$, $\gamma>1$ (nonlinear depletion kinetics). When $\mu=0$, no anomalous diffusion was observed for any choice of k in $t\in[0,\infty)$. This result is consistent with the Boltzmann-Matano theory, but it disagrees from the observations of Kuntz and Lavallée [2]. The most intriguing results are connected with the case $\mu>0$, as clearly reported in Figure 1.
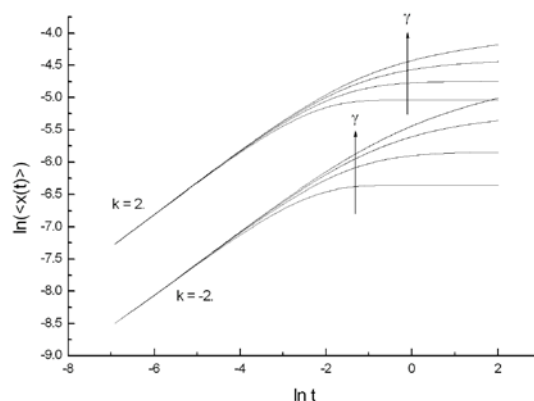

Figure 1. Double logarithmic plot of the moving front position versus time for different values of γ in case of attractive (k= -2) and repulsive (k=2) interactions and $\mu=10$. For each k, from lower to upper curve, γ =1.0, 1.5, 2.0, 2.5.

A crossover time t_c exists, so that a subdiffusive trend appears for $t>t_c$. On the opposite, a classical Brownian-like diffusion with $\alpha=0.5$ holds for $0<t<t_c$, irrespective of both interactions and chemical kinetics.

4. Conclusions

From a methodological point of view, reaction-diffusion processes belonging to the universality class of equations described by Eq.(3) cannot show an anomalous trend of the front propagation at early times ($t\rightarrow 0$) whatever may be the expressions of $D(c)$ and $R(c)$. Such results pose a further limitation of the Fickian approach in data fitting, when a non-classical diffusion is experimentally detected since the first stages of the process. Finally, these findings are confirmed by scaling considerations carried out using an analytical approach. These appealing results may help in tackling with some unresolved problems in engineered materials technology, where the inadequacy of the Fickian approach is still an open problem.

References

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