# Comment on "Scaling Anomalies in Reaction Front Dynamics of Confined Systems"

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In a recent Letter [1], Araujo *et al.* have presented simulations of the reaction-diffusion system $A + B \rightarrow 0$ in one dimension, with initially separated reagents. They find that, for equal diffusion constants, the time dependence of the spatial moments of the reaction profile $R$ are described by a hierarchy of exponents, bounded by the values $\sigma = \frac{1}{4}$ and $\delta = \frac{3}{8}$ describing the temporal scaling of the separation $l_{AB}$ and the midpoint fluctuations $m(t)$ of the neighboring pair of $A$ and $B$ particles. They support the result $\delta = \frac{3}{8}$ by an argument based on the Poissonian fluctuations in the initial state. This behavior contradicts the scaling behavior for $R$ reported elsewhere [2]. In this Comment, I shall argue that fluctuations in the initial state can only give rise to a contribution to $m$ of order $\sim t^{1/4}$, and describe new simulation results that support a scaling hypothesis for $R$ and the distribution $P(m)$ of $m(t)$, with a common time exponent $\approx 0.28 \pm 0.01$, consistent with a slow approach to $\frac{1}{4}$.

To study the effects of the fluctuations in the initial state, consider the difference in densities of the two species $\rho(x,t) \equiv \rho_A - \rho_B$. The equation of motion for $\rho$ for a given initial configuration of particles, averaged over diffusive noise, is a simple diffusion equation. The solution to this equation corresponding to an initial random distribution of $A$ particles for $x < 0$ and $B$ particles for $x > 0$ has only one zero, at $x = x_0(t)$, for $t > 0$. For an ensemble of such initial conditions, with $\overline{\rho(x,0)} = \mathrm{sgn}(x)$, $\overline{\rho(x,0)\rho(y,0)} = \mathrm{sgn}(xy) - \delta(x-y)$ [$\overline{()}$ represents an average over the initial conditions], it can be shown analytically [3] that the probability distribution of $x_0$ as $t \rightarrow \infty$ is of the form $P(x_0) = (w\sqrt{\pi})^{-1} \exp\{-(x_0/w)^2\}$, with $w \sim t^{1/4}$. The argument used by Araujo *et al.* to support $m \sim t^{3/8}$, which is independent of diffusive noise, would also predict $x_0 \sim t^{3/8}$, and so cannot be valid. The origin of its failure will be discussed elsewhere [3].

I have performed simulations of a model similar to the Monte Carlo model of Araujo *et al.* which has no exclusion principle, with similar statistics and equivalent initial conditions, measurement times, etc. I have also performed extended simulations using the probabilistic cellular automata (PCA) model of Ref. [2], whose high efficiency permits higher statistics and longer measurement times. In both cases I confirm $l_{AB} \sim t^{1/4}$, but I find that the quantities $x^{(q)} \equiv \{\int |x|^q R\, dx / \int R\, dx\}^{1/q}$ and $m^{(q)} \equiv \{\int |m|^q P(m)\, dm\}^{1/q}$ both scale as $\sim t^{\beta}$, with $\beta \approx 0.28 \pm 0.01$ independent of $q$. I find that $R(s,t)$ and $P(m)$ are both described well by Gaussian forms, in contrast with Eq. (5) of Ref. [1]. Figure 1 is a plot of $\log_{10} x^{(q)}$ and $\log_{10} m^{(q)}$ vs $\log_{10} t$ for $q = 2$, 8, and 16, from the PCA simulations, for $200 \leq t \leq 102\,400$. The results are for a lattice of size 4000 sites, averaged over 82 176 independent runs, with half of the lattice initially populated at random with $A$ particles, the other half with $B$ particles, with probability of occupancy $\frac{1}{4}$. The straight lines are least-squares fits to the last six data points, whose gradients are all in the range 0.283–0.289. The results of Araujo *et al.* are 0.312, 0.359, 0.367, and 0.375 for $x^{(2)}$, $x^{(8)}$, $x^{(16)}$, and $m^{(q)}$, respectively. The inset shows the gradients between successive points on the log-log plot for $x^{(2)}$, as a function of $1/\log_{10} t$ showing that the effective exponent $d(\log x^{(2)})/d(\log t)$ decreases as $t \rightarrow \infty$, arguably approaching $\frac{1}{4}$. This decrease can be shown to not be due to finite size effects [3].

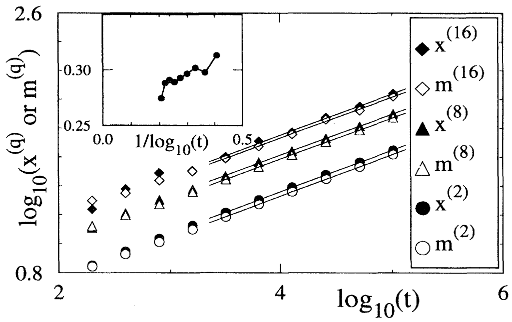


FIG. 1. Plot of $\log_{10} x^{(q)}$ and $\log_{10} m^{(q)}$ vs $\log_{10} t$ for $q = 2$, 8, and 16. Inset: gradients between successive points for $x^{(2)}$, plotted against $1/\log_{10} t$.

In conclusion, the argument predicting $m \sim t^{3/8}$ would appear to be not valid, and this behavior is not reproduced in two independent new sets of simulations. Moreover, the simulations do not support a multiscaling form for $R$, but rather suggest that all relevant length scales behave like $t^{1/4}$ as $t \rightarrow \infty$. I can only conjecture that the results of Araujo *et al.* are an artifact of their simulations.

The simulations referred to in this Comment will be described and discussed in full in a later publication [3]. I would like to thank Michel Droz, Ben Lee, and Hernan Larralde for helpful comments.

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