Comment on "Noise-Induced Bistability in a Monte Carlo Surface-Reaction Model"

In a recent paper, Fichthorn, Gulari, and Ziff[1] report an interesting noise-induced bistability transition in Monte Carlo simulations of the steady state in a heterogeneous catalytic chemical reaction model. We give a mean-field treatment for this model which exhibits this bistability transition and which quantitatively agrees with the simulations of Ref. 1.

The model of Fichthorn, Gulari, and Ziff involves the adsorption and reaction of two immobile species, A and B, and a catalytic substrate. Each microscopic reaction consists of one of the following two events. With probability p_d one particle (either A or B) desorbs, and the unoccupied site is immediately refilled with an A or a B, equiprobably. With the complementary probability $1-p_d$ a nearest-neighbor *pair* of sites is picked, and if these two sites contain an A-B pair, they react and desorb. These unoccupied sites are again refilled with either A's or B's at equal rates. The immediate refilling of empty sites corresponds to the reaction-limited regime, in which particles adsorb readily, but are slow to react. Further details of the process can be found in Ref. 1.

Because the lattice is always full, $n+m=N$, where n is the number of A's, and $m=N-n$ is the number of B's on a lattice of N sites. The catalytic reaction can therefore be represented by a one-dimensional stochastic process in which n changes by ± 1 or 0 at each reaction step. In the mean-field limit, where the distribution of reactants is homogeneous and random, the transition rates arising from the combined influences of reaction and desorption are

$$\begin{aligned}
\mathcal{P}(n\to n+1) &= p_d(1-x)/2+(1-p_d)x(1-x)/2\,, \\
\mathcal{P}(n\to n-1) &= p_d x/2+(1-p_d)x(1-x)/2\,, \qquad (1)\\
\mathcal{P}(n\to n) &= p_d/2+(1-p_d)[1-x(1-x)]\,,
\end{aligned}$$

where $x=n/N$. Taking the continuous approximation of the master equation constructed from these rates yields

$$\begin{aligned}
\frac{\partial}{\partial t}P(x,t) = {} & \frac{p_d}{2}\frac{\partial}{\partial x}[(2x-1)P(x,t)] \\
& +\frac{p_d}{4N}\frac{\partial^2}{\partial x^2}P(x,t) \\
& +\frac{1-p_d}{2N}\frac{\partial^2}{\partial x^2}[x(1-x)P(x,t)]\,, \qquad (2)
\end{aligned}$$

where $P(x,t)$ is the probability that the concentration of A's at time t equals x, and physical time units are used. (One event corresponds to $\Delta t \propto 1/N$.) Desorption leads to both a diffusive and a drift term, the latter tending to drive the system toward equal concentration of A's and B's, $x=\frac{1}{2}$. The reaction process gives rise to a diffusive term, with an associated diffusion constant proportional to $x(1-x)$.

The stationary solution to Eq. (2) is

$$P_\infty(y)=P(y,t\to\infty)=P_\infty(0)[1-(y/y_0)^2]^{-\alpha}\,, \qquad (3)$$

where $y=2x-1$, $y_0=[(1+p_d)/(1-p_d)]^{1/2}$, and $\alpha=[1-(N+1)p_d/(1-p_d)$. For larger desorption rates, $P_\infty(y)$ is peaked at $y=0$, the stable value of the noiseless system, while for $p_d\to 0$, there is a transition to bistability in which $P_\infty(y)$ is peaked near $y\pm 1$ (Fig. 1, compare with Fig. 2 in Ref. 1). Note that for $N\to\infty$ the bistability disappears, as observed in Ref. 1.

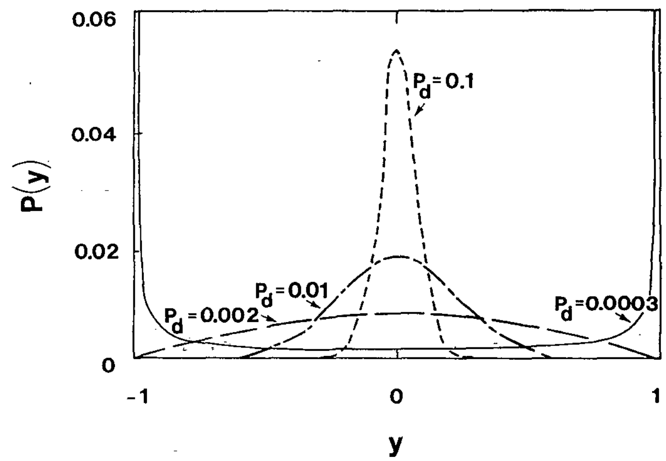

FIG. 1. Plot of the normalized steady-state occupation density, $P_\infty(y)$, as a function of concentration y, for $p_d=0.1$, 0.01, 0.002, and 0.0003, where $N=(32)^2$.

Thus our mean-field approach reproduces the same bistability transition as that observed by Fichthorn, Gulari, and Ziff. Further details will be presented in a forthcoming publication.

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[1]Kristen Fichthorn, Erdogan Gulari, and Robert Ziff, Phys. Rev. Lett. 63, 1527 (1989).

