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Simulations of a monomer-dimer catalysis model on a Sierpinski gasket

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We report results of numerical simulations for a generalized monomer-dimer catalysis model on a Sierpinski gasket. We indicate the existence of a steady-state region, which is much thinner than in the case of the two-dimensional square lattice, although the shape of the phase diagram is the same. In the adsorption-limited case the critical exponents are in good agreement with those obtained for two dimensions. The critical dimension for the monomer-dimer catalysis model is inferred to be 1.

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The monomer-dimer catalysis model was introduced by Ziff, Gulari, and Barshad [1] and later generalized by ben-Avraham *et al.* [2] as a model of carbon dioxide oxidation on a metal catalyst. In the model, the catalysis involves two elementary steps: adsorption and surface reaction. In the adsorption step, which takes place with probability $1-r$, a deposition attempt is made either by an oxygen dimer (A_2) or a carbon monoxide monomer (B) with relative probability p or $q=1-p$, respectively. In the case of A_2 deposition attempt a pair of nearest-neighboring sites is chosen at random and, if both of them are free, they become occupied by (immobile) surface atomic oxygens, which we denote by A_s. In the case of the monomer deposition attempt, a site is chosen at random and if it is free it becomes occupied by surface-bound reactant B_s. In the reaction step, taking place with probability r, a pair of nearest-neighboring sites is chosen at random, and if it is occupied by A_s and B_s, these two reactants bond to form a carbon dioxide molecule which desorbs immediately. This leaves behind two vacant sites which can then accommodate additional particles.

The most interesting feature of the model is the existence of a well-defined region of r and p values where the system can reach a steady state corresponding to continuous reaction [1,2]. Outside this region the catalyst surface eventually becomes fully covered with one of the species (A_s or B_s) and no more reaction is possible. In the case of transition from the A-saturated surface to the steady-state region, concentrations on the surface are changing continously (second-order transition); in the case of transition from the B-saturated surface to the steady-state region, concentrations are changing in a discontinuous manner (first-order transition).

For the adsorption-limited case ($r=1$) extensive numerical simulations were reported by Meakin [3], who confirmed the existence of a steady-state region for the reaction on a square lattice, and reported the existence of a steady-state region for a hexagonal lattice and for long strips with periodic boundary conditions (if the width is greater than 2). Complete phase diagram for the monomer-dimer catalysis model on a square lattice was provided (numerically) by Considine, Takayasu, and Redner [4], who indicated the possibility of the existence of a tricritical point, in the vicinity of which all three regimes (A saturated, B saturated, and steady state) could be observed. A mean-field approach introduced by Considine, Takayasu, and Redner [4] allowed them to describe quantitatively the second-order transition line and qualitatively the first-order transition line, although it did not predict the existence of the tricritical point.

The goal of the current paper is to investigate the case of reaction on a fractal object with dimensionality between 1 and 2. We have chosen a Sierpinski gasket (Fig. 1) because each site of the Sierpinski gasket (except three sites corresponding to the vertices of the enclosing trian-

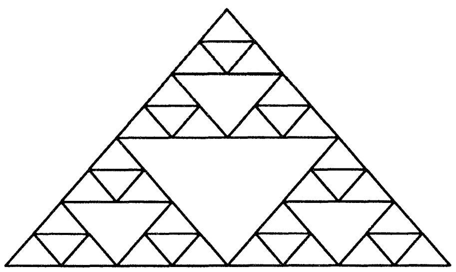

FIG. 1. Sierpinski gasket (iteration 3).

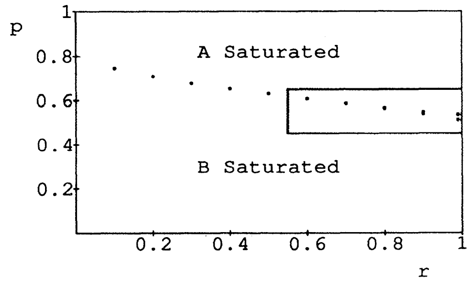

FIG. 2. Phase diagram for the monomer-dimer catalysis model on a Sierpinski gasket. The region where the steady state has been located is highlighted with a box.

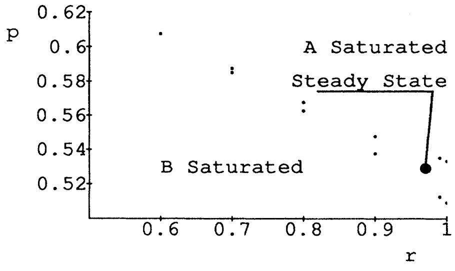

FIG. 3. Enlarged phase diagram for the steady-state region in Fig. 2.

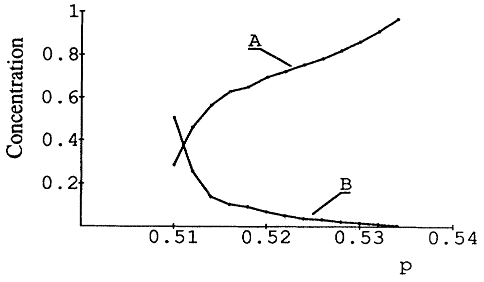

FIG. 4. Concentrations of dimer (A) and monomer (B) covered sites of the catalyst surface in the steady-state region in the adsorption-controlled limit ($r=1$).

gle) has four nearest neighbors, which makes it equivalent to the square lattice from the point of view of the mean-field theory [4].

We performed our simulations on a Sierpinski gasket approximated by a lattice obtained by making eight iterations of the usual transformation, leading to the true Sierpinski gasket in the infinite number of iterations limit. The eighth iteration contains 9843 sites available for adsorption. In order to check the system size dependence, we ran several simulations on the ninth iteration of the Sierpinski gasket (29 526 sites), and no significant difference was detected.

To obtain the phase diagram for a given value of r, a mesh of p values was examined with spacing 0.0025 for $r<1$ and spacing 0.001 for $r=1$. The steady state was judged to exist if the number of steps per lattice site exceeded 1000 without reaching the A-saturated or B-saturated state. When this number is increased by a factor of 2, we confirmed that the transition points do not change. Also no systematic changes are found in concentrations of A_s or B_s at the values of p and r belonging to the steady-state region according to our definition.

The phase diagram we obtained is shown in Figs. 2 and 3. We were not able to locate steady state for the values of r less than 0.6. For $r>0.6$ the steady-state region appears for a small interval of p values, the interval becomes wider as we are closer to the adsorption-controlled limit, but it is still much thinner than in the case of the square lattice [4]. At $r=1$ we have the first-order transition at $p_1=0.509$ and the second-order transtion at $p_2=0.534$ (for the square lattice corresponding values are [3] $p_1=0.4723$ and $p_2=0.6125$).

According to Meakin [3], critical exponents (at $r=1$) for the concentrations of A_s and B_s near the second-order transition are $\beta_A=0.61$ and $\beta_B=0.69$, respectively, and are the same for the square lattice and for hexagonal lattice in two dimensions. Our data (Fig. 4) indicate that $\beta_A=\beta_B=0.7\pm0.1$ for the Sierpinski gasket. It looks probable that the Sierpinski gasket and two dimensions fall into the same universality class.

The mean-field approximation [4] gives a quantitatively good prediction for the second-order transition line in the case of the square lattice. According to the mean-field approximation, which takes into account only the nearest neighbors, the Sierpinski gasket is equivalent to the square lattice and the phase diagrams must be the same. Our results indicate that the mean-field approximation is valid for the Sierpinski gasket only qualitatively, in the sense that the steady-state region does exist as predicted by the mean-field theory, with the exception of the transition point at $r=0$ ($p=0.8$), which is quantitatively correct. That is not the case for the one-dimensional system (line of sites) where the absence of the steady state was demonstrated numerically by Meakin [3]. Our results indicate that the critical dimension for the monomer-dimer catalysis model is definitely less than 2 and probably 1. This supports the prediction [2] that the monomer-dimer process is completely different from the monomer-monomer process for which the critical dimension is believed to be 2.

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