Critical behaviour of the irreversible phase transitions of a dimer-monomer process on fractal media

1994 J. Phys. A: Math. Gen. 27 431

(http://iopscience.iop.org/0305-4470/27/2/026)

J. Phys. A: Math. Gen. 27 (1994) 431–436. Printed in the UK

Critical behaviour of the irreversible phase transitions of a dimer–monomer process on fractal media

Ezequiel V Albano

Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), Facultad de Ciencias Exactas, Universidad Nacional de La Plata. Sucursal 4, Casilla de Correo 16, (1900) La Plata, Argentina

Received 19 April 1993, in final form 1 October 1993

Abstract The dynamic critical behaviour of a dimer–monomer surface reaction process (the ZGB model) of the type $\frac{1}{2}A_2+B\rightarrow AB$ is studied on two different fractals, namely a Sierpinski carpet and percolating clusters, which have almost the same fractal dimension $D_F\cong1.89$. In both surfaces, the model exhibits two continuous irreversible phase transitions. For the Sierpinski carpet the values of the critical exponents interpolate between those of directed percolation in 1+1 and 1+2 dimensions. Results corresponding to percolating clusters are not conclusive enough to assign the universality class of the model.

1. Introduction

Irreversible phase transitions (IPTs) occurring in surface reaction processes have been studied intensively during the last few years. Among others, the model proposed by Ziff, Gulari and Barshad (ZGB) [1] for the dimer–monomer process of the type $\frac{1}{2}A_2+B\rightarrow AB$; which may apply to the oxidation of carbon monoxide [2], i.e. $B\equiv CO$, $A_2\equiv O_2$ and $AB\equiv CO_2$; has received considerable attention [1–16]. The impingement rates of the reactants are always normalized so that $p_A+p_B=1$. B-species arrive to the surface at rate p_B and adsorb if they encounter a vacant site. A_2-molecules arrive at a rate $1-p_B$, and adsorb if they encounter a nearest-neighbour pair of vacant sites. A and B-species adsorbed at neighbouring sites react instantly to form AB, which desorbs leaving two vacant sites on the surface. Therefore p_B is the only parameter of the model. The most distinctive features of this model, as studied using homogeneous two-dimensional surfaces with fractal dimension $D_F=2$, are as follows: a second-order (continuous) IPT from a reactive steady state to an A-poisoned state as p_B drops below $p_{1B}\cong0.389$ [1, 3]; and a first-order (discontinuous) IPT to a B-poisoned state as p_B increases above $p_{2B}\cong0.525$ [1, 4, 5]. Further details on the ZGB model do not need to be repeated here since they have been published previously [1–16].

Meakin *et al* [3] have simulated the ZGB model in one dimension ($D_F=1$), showing that the finite width reaction window between the critical points p_{1B} and p_{2B}, found in two dimensions, collapses into a zero width reaction window for $D_F=1$. Simulations performed using incipient percolating clusters ($D_F\simeq1.89$) as substrata also show the existence of a finite reaction window between poisoned states, but unlike the results obtained for $D_F=2$ the IPT at p_{2B} becomes of second order [9–12]. The ZGB model simulated on a Sierpinski carpet ($D_F\simeq1.89$) also exhibits two second order IPTs, but the critical points are different from those reported for a percolating cluster of almost the same fractal dimension [13]. The existence of the second-order IPT at p_{2B} in the Sierpinski carpet is under debate since Mai *et al* [14] reported a first-order IPT.

It is known that the continuous IPT of the ZGB model belongs to the same universality class as directed percolation (DP) or Reggeon field theory [15, 16]. So far it seems that the critical behaviour of the model depends solely on the dimensionality. Motivated by this evidence Jensen [17] has studied, on the Sierpinski carpet, a simple one-component lattice model with spontaneous annihilation and autocatalytic creation of particles. Dynamic critical exponents obtained on Sierpinski carpets ($1 < D_F < 2$) and reported by Jensen [17] interpolate very nicely between the values corresponding to one- and two-dimensional lattices. This results suggests that continuous IPTs belong to the universality class of $D_F + 1$ *DP* [17].

Based on these results, the purpose of the present work is to determine dynamic critical exponents of the two continuous IPTs exhibited by the ZGB model on both the Sierpinski carpet, i.e. the same substratum used by Jensen [17], and incipient percolating clusters. This study would allow us to find out the universality class of the transitions. Interest in this study also arises from the fact that both fractals have almost the same fractal dimension ($D_F \simeq 1.89$) but, on the one hand the Sierpinski carpet is a deterministic structure while on the other hand an incipient percolating cluster is a random aggregate [18] and consequently they have different physical and geometrical properties,.

2. Dynamic critical behaviour

It has been demonstrated that a fruitful way to test the universality class of irreversible reaction systems is to evaluate exponents related to the time-dependent critical behaviour of the process [4, 5, 16, 17]. The basic idea is to start from configuration closest to the poisoned state and then follow the time evolution of the system. For this purpose we begin with the fractal lattices completely covered with A (B)-species close to p_{1B} (p_{2B}), respectively, except for a blob of empty sites. In fact, due to the disordered structure of the substratum a group of N_e empty sites, with $2 \leqslant N_e \leqslant 9$, are selected close to the centre of the cluster.

The measured quantities are: (i) the survival probability $S(t)$, that is, the probability that the sample was not poisoned after t time steps; and (ii) the average number of empty sites $N(t)$. Lattice sizes are selected large enough to avoid empty sites arriving at the boundary, that is $L=243$ and $L=100$ for Sierpinski carpets and percolating clusters, respectively. Averages are taken over 5×10^4 different samples and runs are performed up to $t = 5 \times 10^3$. Further details on this kind of time-dependent simulation can be found in references [4, 5, 16, 17].

Just at the critical point it is expected that the following scaling laws should hold [4, 5, 16, 17]

$$S(t) \propto t^{-\delta} \tag{1}$$

and

$$N(t) \propto t^{\eta}. \tag{2}$$

Therefore, within the asymptotical regime, log–log plots of $S(t)$ and $N(t)$ versus t will exhibit a straightline behaviour at the critical point. The curves will show curvature when p_B is different from the critical value. This fact makes it possible to obtain precise estimates of p_{1B} and p_{2B} [4, 5, 16, 17].

3. Results and discussion

Results are obtained by means of Monte Carlo simulations in the square lattice of side $L=243$ ($L=100$) and averages are taken over 5×10^4 (1×10^4) different samples for Sierpinski carpets (percolating clusters), respectively. In spite of the fact that fluctuations of the measured quantities should be larger for reactions on percolating clusters, results for these surfaces have poorer statistics because the generation of such clusters is quite time consuming.

Figure 1(a) and 1(b) show log–log plots of $S(t)$ and $N(t)$ versus t, respectively. Results are shown for the Sierpinski carpet at $p_{1B}\simeq0.3815$ and percolating clusters at $p_{1B}\simeq0.344$. The log–log plot of $N(t)$ versus t for percolating clusters at $p_B=0.343$ ($p_B=0.345$) veers downward (upward), respectively, suggesting $p_{1B}\simeq0.344\pm0.001$. Nevertheless, from figure 1(b) it follows that the asymptotic behaviour of $N(t)$ for percolating clusters can hardly be appreciated in spite of the fact that data is taken up to $t=5\times10^3$. So, for this case η has been estimated within the interval $1\times10^3\leqslant t\leqslant5\times10^3$. The estimates of δ and η are shown in table 1.

Results for $S(t)$ and $N(t)$ obtained for the Sierpinski carpet at $p_{2B}\simeq0.4485$ and percolating clusters at $p_{2B}\simeq0.3740$ are shown in figures 2(a) and 2(b), respectively. The estimates of δ and η are shown in table 1. Determination of both the critical point and the critical exponents is more difficult in simulations of the ZGB model on percolating clusters than on the Sierpinski carpet. This fact could be due, on the one hand, to the lack of appropriate statistics and on the other hand, because the asymptotic regime is only reached after longer times. The behaviour of δ at p_{2B} for percolating clusters is quite surprising because at early times one obtains $\delta\simeq0.38\pm0.02$, i.e. a value which is in agreement with previously determined exponents (see table 1). Nevertheless, for $t\geqslant1\times10^3$ the curve can be well fitted by $\delta\simeq0.16\pm0.01$, i.e. a value which may correspond to DP in 1+1 dimensions.

4. Conclusions

The exponents δ and η for the ZGB model simulated on the Sierpinski carpet and for both IPTs are in good agreement with the values reported by Jensen [17] for a one-component model on the same fractal (see table 1). Furthermore, the exponents interpolates between those characteristic of DP in 1+1 and 2+1 dimensions. On the other hand, results obtained simulating the ZGB model on random fractals (percolation clusters) which have almost the same fractal dimension as the Sierpinski carpet are not conclusive enough to determine if the universality class of the model solely depends on the fractal dimension of the underlaying surface. In spite of this shortcoming, the results show that the first-order IPT of the ZGB model at p_{2B} characteristic of $D_F=2$, becomes of second order for $D_F\cong1.9$. Further extensive simulations will be necessary in order to determine more precisely the critical exponents of both continuous IPTs of the ZGB model on the random fractal.

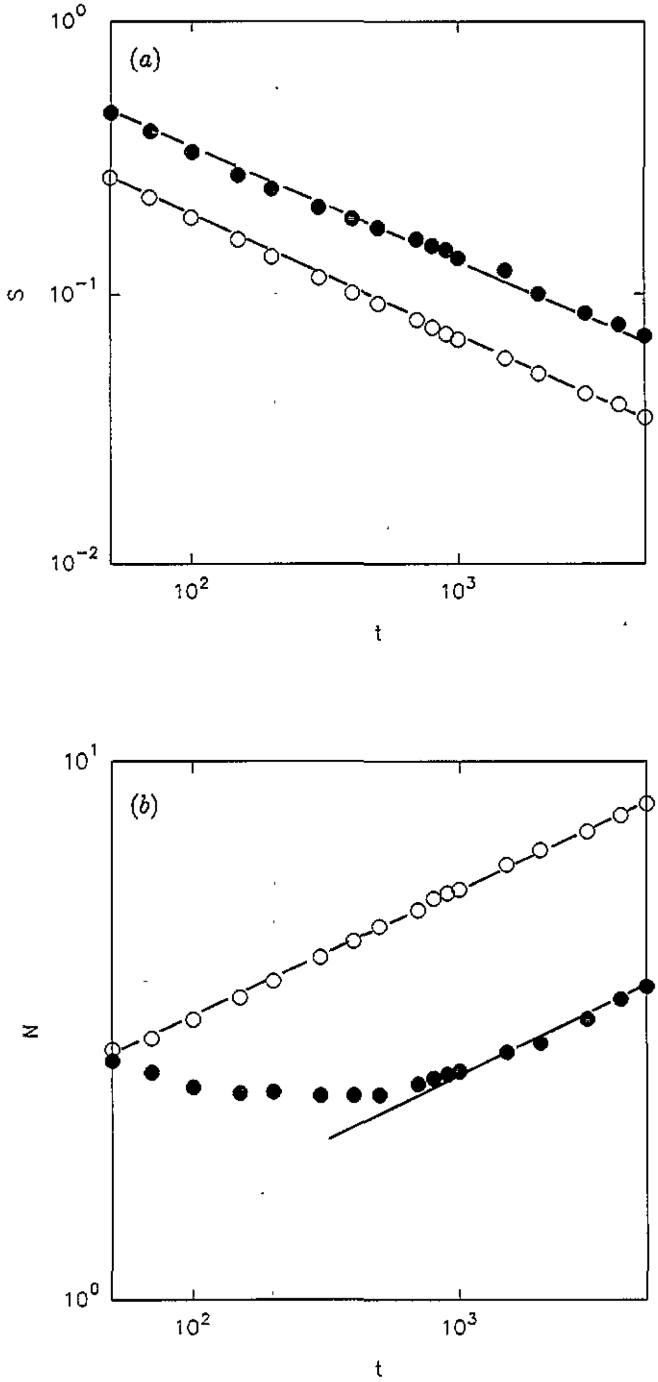

Figure 1. Log–log plots of $S(t)$ (a) and $N(t)$ (b) versus t. Results are shown for the Sierpinski carpet (○) at $p_{1B}=0.3815$ and percolating clusters (●) at $p_{1B}=0.3440$.

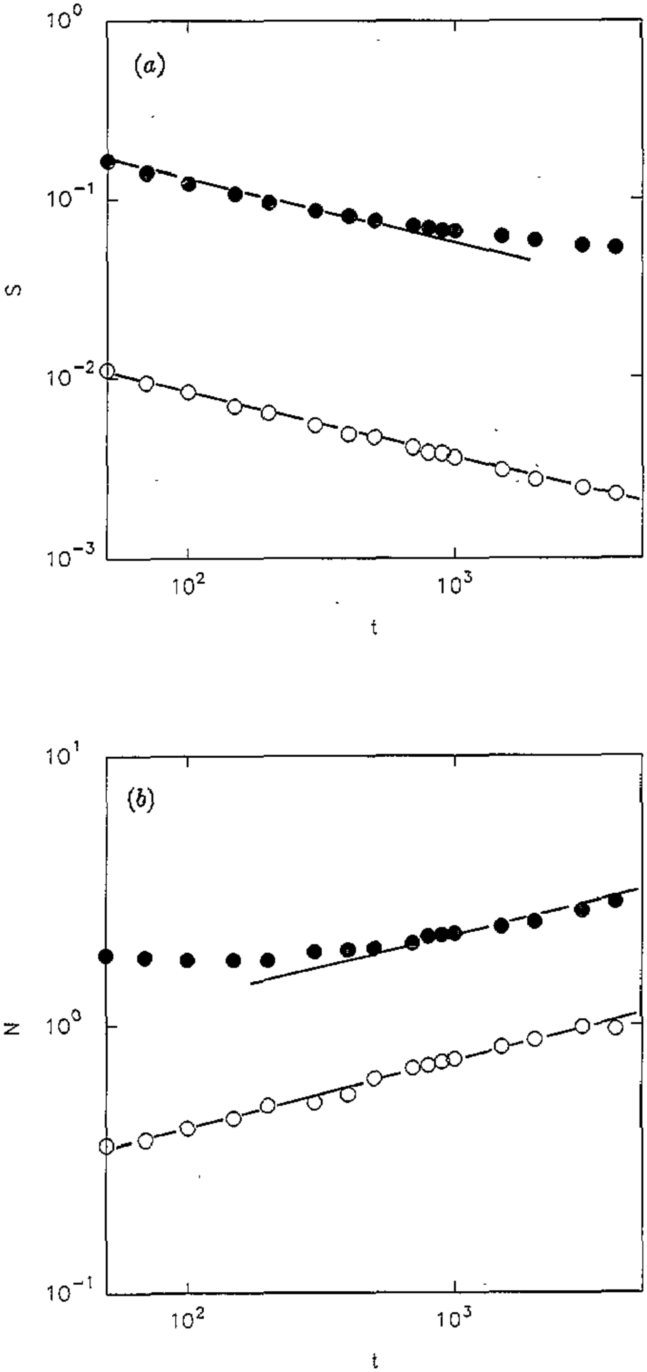

Figure 2. Log–log plots of $S(t)$ (*a*) and $N(t)$ (*b*) versus t. Results are shown for the Sierpinski carpet (○) at $p_{2B}=0.4485$ and percolating clusters (●) at $p_{2B}=0.3740$.

Table 1. List of critical exponents δ and η defined according to equations (1) and (2), respectively. DP ≡ directed percolation in 2+1 and 1+1 dimensions, SC ≡ Sierpinski carpet, IPC ≡ incipient percolating clusters, IC ≡ one-component model of Jensen [17] and PW ≡ present work. (a) and (b) corresponds to estimations of δ for $t<10^3$ and $t>10^3$, respectively. For the PW, error bars merely reflect the statistical errors of the least square fits.

Model	δ	η	References
DP in $(1+1)D$	0.162 ± 0.004	0.317 ± 0.002	18
ZGB on IPC at p_{1B}	0.41 ± 0.02	0.23 ± 0.01	PW
ZGB on IPC at p_{2B}	0.38 ± 0.02 (a)	0.20 ± 0.02	PW
ZGB on IPC at p_{2B}	0.16 ± 0.02 (b)		PW
ZGB on SC at p_{1B}	0.43 ± 0.01	0.23 ± 0.01	PW
ZGB on SC at p_{2B}	0.38 ± 0.01	0.24 ± 0.01	PW
IC on SC	0.400 ± 0.010	0.235 ± 0.010	17
ZGB on $2D$	0.452 ± 0.008	0.224 ± 0.010	16
DP in $(2+1)D$	0.460 ± 0.006	0.214 ± 0.008	19

Acknowledgments

This work was supported by the CONICET (Argentina). The Alexander von Humboldt Foundation (Germany) and Fundación Antorchas (Argentina) are greatly acknowledged for the provision of valuable equipment.

References

[1] Ziff R M, Gulari E and Barshad Y 1986 *Phys. Rev. Lett.* **56** 2553
[2] Ehsasi M, Matloch M, Frank O, Bloch J H, Chrismann K, Rys F S and Hirschwald W 1989 *J. Chem. Phys.* **91** 4949
[3] Meakin P and Scalapino D J 1987 *J. Chem. Phys.* **87** 731
[4] Evans J W and Miesch M S 1991 *Phys. Rev. Lett.* **66** 833
[5] Evans J W and Miesch M S 1991 *Surf. Sci.* **245** 401
[6] Evans J W 1991 *Langmuir* **7** 2514
[7] Chopard B and Droz M 1988 *J. Phys. A: Math. Gen.* **21** 205
[8] Yaldran K and Sadiq A 1989 *J. Phys. A: Math. Gen.* **22** 1925
[9] Albano E V 1990 *J. Phys. A: Math. Gen.* **23** L545
[10] Albano E V 1990 *Phys. Rev. B: Rapid Commun.* **42** 10818
[11] Albano E V 1990 *Surf. Sci.* **235** 351
[12] Albano E V 1991 *J. Chem. Phys.* **94** 1499
[13] Albano E V 1992 *Phys. Lett.* **168A** 55
[14] Mai J, Casties A and von Niessen W 1992 *Chem. Phys. Lett.* **196** 358
[15] Grinstein G, Lai Z W and Browne D A 1989 *Phys. Rev.* A **40** 4820
[16] Jensen I, Fogedby H C and Dickman R 1990 *Phys. Rev.* A **41** 3411
[17] Jensen I 1991 *J. Phys. A: Math. Gen.* **24** L1111
[18] Stauffer D and Aharony Y 1992 *Introduction to Percolation Theory* (London: Taylor & Francis) 2nd edn
[19] Grasberger P 1989 *J. Phys. A: Math. Gen.* **22** 3673