Static and dynamical critical behavior of the monomer–monomer reaction model with desorption

E.C. da Costa *, Flávio Roberto Rusch

Departamento de Física - Centro de Ciências Tecnológicas - UDESC, 89219-710, SC, Brazil

HIGHLIGHTS

- The monomer–monomer reaction model ($A + B \rightarrow AB$) in the linear chain. The B monomer desorbs with probability α.
- The model displays a continuous phase transition from an absorbing phase into a reactive steady state.
- The critical behavior was studied by mean field theory (site and pair approximations) and Monte Carlo simulations.
- The model exhibits the same critical exponents of the directed universality class.

ARTICLE INFO

ABSTRACT

We studied in this work the monomer–monomer reaction model on a linear chain. The model is described by the following reaction: $A + B \rightarrow AB$, where A and B are two monomers that arrive at the surface with probabilities y_A and y_B, respectively, and we have considered desorption of the monomer B with probability α. The model is studied in the adsorption controlled limit where the reaction rate is infinitely larger than the adsorption rate. We employ site and pair mean-field approximations as well as static and dynamical Monte Carlo simulations. We show that the model exhibits a continuous phase transition between an active steady state and an A-absorbing state, when the parameter y_A is varied through a critical value, which depends on the value of α. Monte Carlo simulations and finite-size scaling analysis near the critical point are used to determine the static critical exponents β and $\nu_\perp$ and the dynamical critical exponents $\nu_\parallel$ and z. The results found for the monomer–monomer reaction model with B desorption, in the linear chain, are different from those found by E. V. Albano (Albano, 1992) and are in accordance with the values obtained by Jun Zhuo and Sidney Redner (Zhuo and Redner, 1993), and endorse the conjecture of Grassberger, which states that any system undergoing a continuous phase transition from an active steady state to a single absorbing state, exhibits the same critical behavior of the directed percolation universality class.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Since the pioneering work of Schlögl [1] and Ziff, Gulari and Barshad [2] statistical mechanics community has made great progress in the study of chemical reaction on a catalytic surface [3], nonequilibrium phenomena [4] and in stochastic dynamics and irreversibility [5]. Examples of recent problems on nonequilibrium processes include markets [6,7], rain precipitation [8], sandpiles [9] and conserved contact process [10]. There is also a great interest in modeling interface

* Corresponding author.
E-mail address: edio.costa@udesc.br (E.C. da Costa).

growth [11,12], traffic flow [13], temperature dependent catalytic reactions [14], predator–prey systems [15], population dynamics [16] and epidemic models [17]. Nonequilibrium magnetic systems, with a well defined hamiltonian, have been also studied in the context of nonequilibrium processes [18,19] as well. Until now, we do not have a complete theory accounting for the nonequilibrium systems although stochastic approach to equilibrium and nonequilibrium thermodynamics, using the master equation and the Fokker–Planck equation has been done. To this we recommend the recent work done by Tânia Tomé and Mário J. de Oliveira [20]. The fundamental concept of a Gibbsian distribution of states in equilibrium has no counterpart in the nonequilibrium situation. This happens because many of these systems do not present even a hamiltonian function and, if it is possible to define a hamiltonian, the detailed balance would be violated.

For the equilibrium systems we can induce phase transitions by changing some external parameters. Usually, the temperature is the selected control parameter to study phase transitions between equilibrium states. In the case of continuous phase transitions, at the critical point, long range correlations are established inside the system and a set of critical exponents can be defined to describe the critical behavior of some thermodynamic properties. The renormalization group theory [21] is a well known theory that allows the calculation of these critical exponents.

We can also consider external constraints for the nonequilibrium systems that can drive the dynamical behavior of the system. The nature of the external parameter depends on the nature of the system. For instance, in an epidemic model for the spread of a disease, the external parameter to be considered is the rate of change of the healthily individuals into unhealthily ones. In a catalytic reaction model, the external parameter can be the rate of change of the concentration of reactants. These, and many other examples of nonequilibrium systems display dynamical phase transitions. A comprehensive survey on the dynamic phase transitions and nonequilibrium systems can be found in the books of Marro and Dickman [4] and Privman [22].

Catalytic reaction models are a class of nonequilibrium systems that show phase transitions among its stationary states, particularly, these are irreversible phase transitions (IPT) and many other catalytic reaction models appeared in literature [23].

The monomer–monomer reaction model [24,25] is the simplest catalytic reaction model, described by the reaction $A + B \rightarrow AB$, where A and B are two monomers that arrive on a surface with probabilities y_A and $y_B = 1 - y_A$, respectively. This model was studied in the reaction controlled limit as well as in the adsorption controlled limit. In both cases, if $y_A > 0.5$, the surface becomes saturated by monomers A, and the system always enters into an absorbing state. On the other hand, if $y_A < 0.5$, the absorbing state is one in which the lattice is completely covered by monomers of the type B. However, if $y_A = 0.5$, the surface still saturates but with a much slower rate, and there is no preferred species to saturate the catalyst. The mapping onto the kinetic Ising model [26] showed that the time for the system to enter the absorbing state, at the particular value $y_A = 0.5$ and, in the reaction controlled limit, grows with the system size. Studies including monomers with different sizes [27], substrate viewed as a complete graph [28], introduction of a repulsive interaction between like monomers [29], the increase in the number of degrees of freedom for the reaction [30], are some examples of the research concerning the monomer–monomer reaction model. In 1992, E. V. Albano [31] studied the monomer–monomer reaction model using Monte Carlo technique employing three different substrate: one and two dimensional lattices, and incipient percolation clusters in two dimensions. He considered B desorption with probability one and conclude that this monomer–monomer reaction model does not belong to the Reggeon Field Theory (RFT), that is, the Direct Percolation (DP) universality class. However, Jun Zhuo and Sidney Redner [32] used series expansion [33] to provide evidence that the critical exponents of Albano's model in one dimension agree with those of DP. The DP universality class is the paradigm to describe the nonequilibrium phase transitions of a variety of models. However, the experimental determination of the critical exponents is too hard. In real systems, a perfect absorbing state is not easily realized because there are always small fluctuations, for instance, due to thermal desorption of the elements. The presence of impurities, inactive sites and other inhomogeneities on the catalyst also difficult the measurements of the critical exponents. A full account on the possible experimental realizations of Direct Percolation can be found in the review work of Hinrichsen [34] and the references therein, as well as in the work done by Kazumasa and co-authors [35].

In the present work we considered the monomer–monomer reaction model with B desorption with probability α. The catalyst was represented by a linear lattice, and it is in contact with an infinite reservoir of monomers A and B in their gaseous phases. The monomers A and B arrive at the surface with probabilities y_A and $y_B = 1 - y_A$, respectively. These probabilities are related to the partial pressures of the gases A and B inside the reservoir. The model was investigated by effective field approximations, as well as through static and dynamic Monte Carlo simulations in $d = 1$ dimension. The model also exhibits continuous phase transition into an absorbing state, and the finite-size scaling arguments show that the model belongs to the same universality class of the Directed Percolation for all the values considered to the parameter α.

This paper is organized as follows: in the next section we describe the model and we present the results obtained through the site and pair mean-field approximations. In Section 3 the model is studied by using static Monte Carlo simulations and finite-size scaling arguments. Section 4 is dedicated to the study of the dynamical critical behavior of the model. In the last section we present our main conclusions.

2. Model and mean-field approximations

We consider a catalytic surface in contact with an infinite reservoir of monomers, labeled by A and B. The catalyst will be represented by a linear chain. These monomers can be adsorbed onto the lattice, and they can react according to the