Comment on “Critical Exponents for the Irreversible Surface Reaction \( A + B \rightarrow AB \) with B Desorption on Homogeneous and Fractal Media”

Recently, Albano [1] found that the monomer-monomer catalysis model with one species (B) allowed to desorb exhibits a second-order transition from the reactive to the A-saturated state which does not belong to the Reggeon field theory (RFT) universality class. This is surprising, as the universality class of RFT is believed to encompass almost all models which exhibit a continuous phase transition to a single absorbing state [2]. Here, we use series expansions [3] to provide evidence that the critical exponents of Albano’s model in one dimension agree with those of RFT.

In the adsorption-controlled limit, the model is defined as follows:

\[
A + S \xrightarrow{k_d} A_S, \quad B + S \xrightarrow{k_d} B_S,
\]

\[
A_S + B_S \xrightarrow{k_d} (AB)_S \uparrow + 2S.
\]

Here S denotes a surface site and \( X_S \) denotes an adsorbed species. The evolution operator \( \mathcal{O} \) of the system is given by [3] \( \mathcal{O} = \rho(\mathcal{A}_B - \mathcal{A}_A) + (\mathcal{A}_A + \rho \mathcal{D}_B) \), where \( \mathcal{A}_X \) is the operator for adsorption and subsequent reaction for species \( X \).

\( \mathcal{D}_B \) is the desorption operator for \( B \)'s, \( \rho = k_d/(k_d+k_b) \), and \( r = k_d/(k_d+k_b) \). (Albano [1] investigated the special case \( r = 1 \).) Given a configuration \( \gamma \) with \( n_E \) empty sites and \( n_B \) B’s, \( \mathcal{A}_A(\gamma) = \sum_{\gamma'}(1)(\gamma') \), \( \mathcal{A}_B(\gamma) = \sum_{\gamma'}(2)(\gamma') \), \( \mathcal{A}_A(\gamma) = \sum_{\gamma'}(1)(\gamma') = n_E(\gamma) \), and \( \mathcal{A}_B(\gamma) = \sum_{\gamma'}(2)(\gamma') = n_B(\gamma) \), where \( (\gamma') \) and \( (\gamma'') \) are the configurations generated from \( \gamma \) by the action of \( \mathcal{A}_A \) and \( \mathcal{D}_B \) on \( \gamma \). We performed a small \( p \) expansion up to nineteenth order for various values of \( r \) starting with all sites occupied by \( A \)'s, except for a single vacancy. For example, for \( r = 1 \), the coefficients of the Laplace transform of the average number of empty sites, \( \mathcal{N}_E(s) \), at \( s = 0 \) are

\[
\]

Using differential approximants, our estimates of the critical exponents are in close agreement with RFT (Table I). We also performed a time-dependent Monte Carlo simulation [4] of this model for \( r = 1 \) in one dimension. Our algorithm is as follows: Define \( r' = n_B/(n_E + n_B) \), and pick a random number \( y \). If \( y < r' \) then a randomly selected \( B \) desorbs; otherwise, deposit an \( A \) or a \( B \) on a randomly selected empty site with probability \( p \) or \( 1 - p \), respectively, and remove a reactive pair if one is created. Finally, the time is incremented by \( 1/(n_E + n_B) \). A plot of the local exponent for \( n_E(t) \), \( \eta(t) \), vs. \( 1/t \) is shown in Fig. 1. The exponents estimated from the simulation are \( \delta = 0.16(1) \), \( \eta = 0.29(2) \), and \( z = 1.21(2) \), which once again agree with the values of RFT.

As \( r \rightarrow \infty \), the dynamics of the vacant sites maps exactly to the cluster dynamics of the single-component \( A \) model [3], which is in the RFT universality class. This mapping, together with our numerical evidence suggests that the continuous phase transition from the reactive to the saturated state in the monomer-monomer model with one desorbing species is of the RFT type.

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| TABLE I. Estimates for the critical point and critical exponents for the catalysis model and RFT in 1D. |
|-----------------|-----------------|-----------------|-----------------|
| \( r = 0.5 \)   | \( r = 1 \)     | \( r = 10 \)    | RFT             |
| \( \rho \)       | 0.5915(3)       | 0.6137(1)       | 0.6599(2)       | \ldots         |
| \( \nu(1 - \delta) \) | 1.50(3)         | 1.450(6)        | 1.43(2)         | 1.445          |
| \( \nu(1 + \eta) \) | 2.27(2)         | 2.274(6)        | 2.27(2)         | 2.281          |