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Two dimensional versus one dimensional behavior for biased diffusion and aggregation in a network of channels

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ABSTRACT

We present an extension to two dimensions of a one-dimensional model for a fluid that drags particles in a narrow channel [V. Ruiz Barlett, M. Hoyuelos, H.O. Mártin, Physica A 387 (2008) 4623–4629]. We consider a network of narrow channels on a strip. There is a flux rate J of particles that enter in the left end of the system; particles move to the right, up or down with a jumping rate P. When two particles collide, they produce a cluster that remains immobile because the size of the cluster is greater than the channel diameter. After some time, the accumulation of clusters plugs the system up. We analyze the clogging time against J/P with results obtained from numerical simulations and from a continuous description with approximate differential equations. A transition from a 2D to a 1D behaviour is observed for $J/P \ll 1$. The transition point depends on the value of the number of longitudinal channels in the network, w. For $J/P \gg 1$, we demonstrate analytically, and confirm numerically, that the clogging time behaves as $\ln w$.

1. Introduction

The study of simple models of reaction-diffusion processes has attracted much attention during the last decades not only because they show a very rich dynamical behaviour, but also because they are relevant from the theoretical [1–3] and experimental point of view due to the development of recent observation techniques [4].

We will focus on a reaction-diffusion process where the diffusion is biased, the reaction is coagulation and particles are injected in one extreme of the system. After coagulation takes place, the mobility of the resulting cluster is usually reduced. For simplicity, we will consider that the cluster becomes immobile, since the clusters formed by nucleation have a higher probability to deposit in the system than the individual particles. This kind of process is relevant in the study of a wide variety of systems, e.g. catalyst reactions in porous media [5–8], filters [9], atheromatous plaques in arteries [10,11], and impurity transport in pipes [12].

In Ref. [13], a one-dimensional model with biased diffusion and coagulation reactions was analyzed. Related models of biased diffusion can be found in Refs. [14–16]. The present paper is an extension of Ref. [13] where we consider a two-dimensional model. The model is intended to be a simplified representation of a fluid that drifts impurities through a network of narrow channels on a strip (see Fig. 1). An accumulation of immobile impurities in a given region of the system can plug it up. The aim of the work is to derive and identify qualitative and general behaviours of the system as the relevant parameters are varied, and to analyze the transition between two (2D) and one-dimensional (1D) behaviors. In particular, we are interested in the behaviour of the clogging time and the mean penetration distance as the parameters are varied. The parameters are the input flux rate, the drift rate and the width of the lattice.

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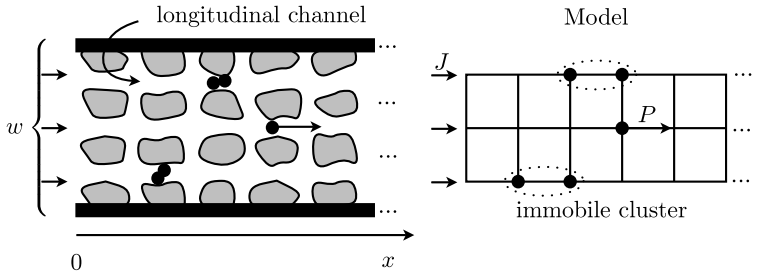

Fig. 1. Schematic representation of a porous medium of finite width w and infinite length; w is the number (mean number) of longitudinal channels of a regular (disordered, respectively) porous medium. The dots represent the impurities that are dragged by a fluid that enters from the left end of the system and moves to the right. The impurities are particles of a size comparable to the channel diameter. When two particles collide they produce a cluster, larger than the individual particles, that cannot move through the medium and remains immobile. This coagulation takes place at any point of the porous network. The right figure shows the lattice that we use as a model to describe the network of channels. For simplicity, in the model the coagulation occurs between two particles located at a nearest-neighbor distance of the square lattice.

The details of the model are described in Section 2. A mean field approach is introduced in Section 3, with which approximate partial differential equations are derived for the densities of mobile and immobile particles. In Section 4 we present the results obtained from a Monte Carlo simulation of the model and from numerical integration of the equations. Finally, the conclusions are stated in Section 5.

2. The model

We have a discrete two-dimensional lattice of $(L+1)\times w$ sites, labeled with indices (i,j) that take values from 0 to L, and from 1 to w, respectively. Particles can enter into the system only in the first column in the left end, that correspond to sites with $i=0$ and $1\leq j\leq w$. The parameters are: the input flux rate J (particles per unit time that enter into each site of the first column), the drift rate P (particles move to the right, up or down nearest-neighbor sites with probability per unit time P) and the width w (the number of narrow longitudinal channels, see Fig. 1). The probability of a left jump is taken equal to zero. Multiple occupancy of sites is not allowed.

For $w=1$, we recover the one-dimensional model analyzed in Ref. [13], where two different regimes were identified: entrance limited regime ($J\ll P$) and diffusion limited regime ($J\gg P$).

Each site of the lattice can be empty or occupied by a mobile or immobile particle. If the first column ($i=0$) is completely occupied by immobile particles, the system becomes clogged or saturated and no further entrance of particles is possible. The number of sites L is large enough so that the system becomes clogged before any particle reaches site L, to avoid finite size effects. We used rigid boundary conditions in the upper and lower limits of the lattice ($j=1$ and $j=w$). We checked that the results obtained do not change if periodic boundary conditions are used.

Initially, the system is empty and the number of mobile particles is $N=0$. Particles can enter into the system in any site of the first column whenever it is empty. A small time scale τ is chosen in order to obtain two numbers, $\epsilon=wJ\tau$ and $p=3P\tau$, smaller than 1, that represent probabilities (probability p corresponds to the combination of the three events: up, down or right jump). A new particle can enter into any empty site of the first column with a probability of ϵ and a mobile particle can move with a probability of p, in a time interval τ.

In each Monte Carlo (MC) step we randomly choose one among $N+1$ particles (there are N mobile particles plus one that is waiting outside the lattice to enter). In one MC step we have the following possibilities:

- If the new particle is chosen, we randomly choose one of the w sites of the first column and, if it is empty, the particle enters with probability ϵ.
- If one of the N mobile particles is chosen, one of the three possible directions (up, down or right) is chosen with a probability of 1/3, and the particle tries to jump with a probability of p. If $j=1$ ($j=w$), the downward (upward) jump is not performed. If the new site is empty, the particle jumps. If the new site is occupied by another mobile particle, both particles react and form an immobile cluster that occupies two sites, and the selected particle remains at its original position. If the new site is occupied by an immobile particle, the jumping particle reacts and transforms to an immobile one, remaining at its original position and forming a bigger cluster.

In each step the time is increased by $\Delta t=\tau/(N+1)$.

3. Continuous description

In this section we present a system of partial differential equations that approximately describes the evolution of the mobile and immobile particle densities of the discrete model described in the previous section.

We define the occupation numbers $s_{i,j}$ and $c_{i,j}$ for mobile and immobile particles respectively; the indexes i and j represent the coordinates of the position in the lattice and take values 0 to L and 1 to w, respectively. These numbers take values 1