# ARTICLES

## Driven diffusion of particles, first-passage front, and interface growth

R. Bidaux

*SPEC, Orme des Merisiers, CE Saclay, 91191 Gif-Sur-Yvette, France*

R. B. Pandey

*The Program in Scientific Computing and Department of Physics and Astronomy,*
*University of Southern Mississippi, Hattiesburg, Mississippi 39406-5046*

We study a computer-simulation model for driven particles on a discrete lattice where a fraction $p$ of the lattice sites is randomly occupied by frozen impurities (barriers), and an imposed bias governs the particles' hopping through the lattice. These particles (the carriers) are initially released from a source of wetting fluid from one end of the lattice in order to wet and the dry lattice on their trails. We study the transport of particles, frontier of their trail, and the growth of the interface between the wet and dry regions as a function of the biased field and the number of carriers. The rms displacements of carriers $(R_{\text{tr}})$ and that of their center of mass $(R_{\text{c.m.}})$ show power-law behaviors with time $t$, with exponents depending on the biased field. At the impurity concentration $p=0.30$ in two dimensions, we find that the mean wetting front position $R_f$ moves with a power law $R_f \sim t^{2/3}$ at low values of the biased field, whereas it becomes pinned at higher values. The interface width grows with time to a maximum value before relaxing to a saturation value.

Understanding the transport of particles in the presence of a biased field [1] and the growth of interface [2,3] via models has attracted a considerable interest in recent years. Growth of interface in deposition of particles (pouring down on a substrate) [4–6] has been extensively studied for a variety of rules regarding a trajectory of particles and their sticking mechanisms. Attempts have been made to relate the results of the computer simulations for the kinetic exponents and scaling with experiments such as the growth of materials, cracks in brittle materials, fluid mixtures, wetting by imbibition, etc. [6,7]. Many issues regarding the relevance of various models with respect to experiments, whether the agreement is excellent or poor, are still a subject of active interest. A common difficulty with experiments, analytical theories, and computer simulations is to make a connection between the experiments and models from their microscopic description to the macroscopic observations. However, one needs to investigate relevant models [6–20] that help in understanding the global properties arising from the microscopic details. In this article we attempt to study such a model.

We consider a discrete lattice (a two-dimensional lattice of size $L_x \times L_y$ here). One end of the lattice, say the first column, is connected to a source of the wetting fluid, i.e., the wetting fluid can emanate from each site of the first column. However, the fluid flows into the dry lattice only via mobile particles, which is a mechanism for the controlled spreading of the fluid into the lattice. Initially,

a fixed number $N_p$ of particles are placed randomly in the first column. In this model of controlled spreading, $N_p$ may vary from 1 to $L_y$, the size of that source column. A fraction $p$ of the lattice sites is randomly occupied by quenched impurities which act as infinite barriers for the particles transport. Thus, the particles are allowed to move only on a fraction $(1-p)$ of the remaining lattice sites. In addition, a biased field is set up which governs the hopping probabilities of the particles to their neighboring sites. These probabilities along $\pm x$ and $\pm y$ directions are given by $B_{\pm x} = (1 \pm B)/4$, where $B$ is the bias factor $0 \le B \le 1$, and $B_{\pm y} = \frac{1}{4}$. From this distribution of the biased field one expects an overall drift of each particle from the source to the bulk of the lattice along the $+x$ direction.

We implement the following procedure for moving the particles and dragging the fluid. A particle at a site $i$ is selected randomly. One of its neighboring sites $j$ is then chosen according to the above-defined biased probabilities. If site $j$ is empty, then the particle is moved from site $i$ to site $j$, and site $j$ becomes wet if it was dry; a wet site remains permanently wet. If site $j$ is forbidden (i.e., if it is an impurity site, or already occupied by another particle), then the particle remains at site $i$. An attempt to move each particle once on average is defined as one Monte Carlo step (MCS) (i.e., unit time). We use periodic boundary conditions along the $y$ direction and a reflecting boundary condition at the source end along the $x$ direc-

tion. The length $L_x$ has been chosen in such a way that no mobile particle can reach the end opposite the source (i.e., the abscissa $L_x$) during the simulation time of interest. As the particles execute their stochastic motion, the fluid spreads on their trail. At this point we would like to mention that the irreversible wetting procedure thus defined may also be viewed as the result of some kind of radioactive marking or more generally as the remanence of an everlasting polluting effect. For a fixed biased probability $B$ and a constant number of carriers $N_p$ we carry out our simulation up to a fixed time. This process is repeated for a large number of independent samples with independent impurity distributions, in order to obtain a reliable average estimate. In each sample, at a given time step $t$, we call the ensemble of wet sites (one per row) the "wetting front," such that each of these sites is, in the row it belongs, the wet site with the largest abscissa. (This definition is conventional although it neglects the possible presence of dry islands.) Within each sample we evaluate the growth of the mean wetting front position $R_f$, the interface width $W$, the root-mean-square (rms) displacement $R_{tr}$ of each particle, and the rms displacement $R_{c.m.}$ of their center of mass, which are defined as

$$R_f = \frac{1}{L_y} \sum_{i=1}^{L_y} x_{if} \, ,$$

$$R_{tr}(x,t) = \frac{1}{N_p} \sum_{i=1}^{N_p} \left[ \frac{1}{t} \sum_1^t x_i^2(t) \right]^{1/2} \, ,$$

$$R_{c.m.}(x,t) = \frac{1}{t} \sum_1^t \left[ \frac{1}{N_p} \sum_{i=1}^{N_p} x_i(t) \right]^2 \, ,$$

where $x_{if}$ is the farthest wet site in the $i$th row and $R_{tr}(x,t)$ and $R_{c.m.}(x,t)$ refer to the $x$ component of the rms displacement of the tracers and that of their center of mass, respectively, at time $t$. Note that $R_{tr}$ describes the motion of each particle while $R_{c.m.}$ describes the collective motion of all particles as a function of time; a particle is also called a tracer and a carrier. The averaging is then performed over all samples. From now on, all the data reported here will take into account the sample averaging. This model is different from a similar study recently presented by Family and Pandey [14] where effects of external bias, quenched barriers, and the variation in the number of carriers are not considered. We believe that incorporating these parameters in our model makes our model more realistic particularly in the case of imbibition experiments [7] such as the spreading of water on a paper towel. Random distribution of the impurity generates an inhomogeneous porous matrix of those sites which are not occupied by the impurities and this may capture some aspects of porous paper towel. The biased field is equivalent to the pressure while a fixed number $N_p$ of carriers models a controlled release of fluid. Although this model does not capture all the details of the laboratory experiments, it incorporates more relevant details than the model presented in Ref. [14].

Figure 1 shows the variation of the mean wetting front position $R_f$ versus time on a log-log scale for various

values of $N_p$ and a biased field at a fixed impurity concentration $p = 0.30$. In the absence of impurities ($p = 0.00$) we should observe a linear power-law dependence of $R_f$ on $t$, i.e., $R_f \sim t$, as expected for the biased diffusion [20]. At a constant biased field $B_{+x} = 0.35$ at $p = 0.30$, we observe a power-law behavior with time, $R_f \sim t^k$ with $k \simeq 0.65 \pm 02$ in the asymptotic regime for a small number of carriers ($N_p = 1,2,4,8$) [Fig. 1(a)]. For $N_p = 16$, the exponent $k$ remains in the same range in most of the time regime (up to 50 000 MCS). For a larger number of carriers, i.e., $N_p = 25$ and 50 with $L_y = 50$, we also observe an excellent asymptotic power law with $k \simeq 0.65$ [Fig. 1(b)]. However, for $N_p = 25$ with $L_y = 25$, we do not see quite as linear a power-law dependence. We attribute this deviation to the finite-size effects: the particles' motion becomes more correlated (essentially due to hard-core repulsion) on increasing the number of carriers. If the correlation length becomes larger than the system's transverse size $L_y$, then the finite-size effects become more important. We would like to point out that in all cases, the $R_f$ versus $t$ plot on the log-log scale exhibits a negative second derivative (i.e., curvature) which goes slowly to zero for long times, making the evaluation of the exponent $k$ somewhat uneasy. One plausible *a pos-*
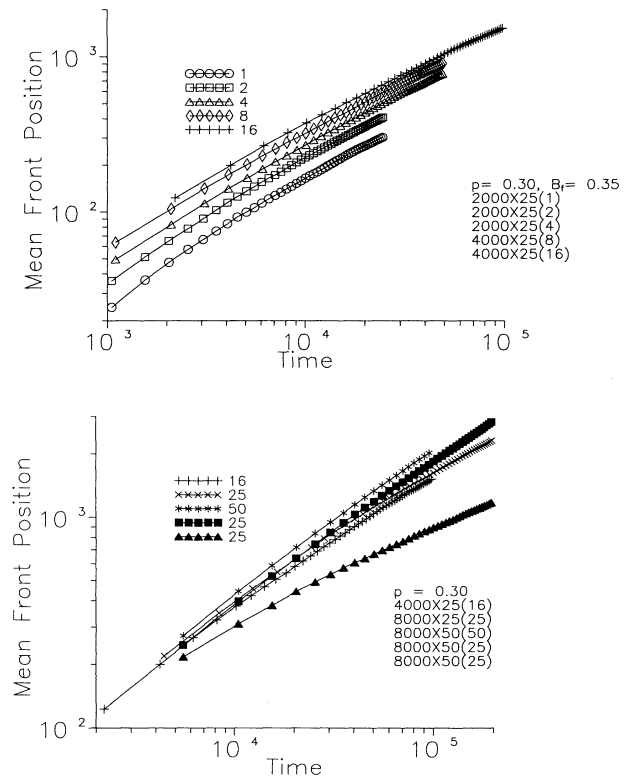


FIG. 1. Mean front position vs time on a log-log scale at a fixed impurity concentration $p = 0.30$. Numbers in parentheses are the values of the number of particles $N_p$. Over 500 independent samples were used for each curve. (a) $N_p = 1$, 2, 4, 8, and 16 for the forward bias $B_{+x} = 0.35$. (b) $N_p = 16$, 25, and 50 with different lengths $L_y = 25$ and 50 for the forward bias $B_{+x} = 0.35$ except the lowest curve, which is with $B_{+x} = 0.40$.

*teriori* improvement would be to assume that $R_f \sim (t - t_0)^k$ where $t_0$ is a relaxation (or transient) time. In $\log(R_f)$-$\log(t)$ coordinates, the corrections to a straight line should be exponential. Due to statistical errors, this possibility is hard to confirm and must be postponed to further studies. The asymptotic value of the exponent $k$ decreases on increasing the bias, and becomes zero at $B_{+x} = 0.50$ when the wetting front is pinned by the impurity barriers. Such pinning is also observed in other biased growth models [16,17] as well as models for fluid flow through porous media [18,19]; in Ref. [19], a critical transition to depinning as a function of driving force is emphasized.

The one-particle case ($N_p = 1$) deserves some comments. Suppose we consider now a finite longitudinal length $l_x$ and ask, how does the average first-passage time $T$ of the particle at the abscissa $l_x$ depend on $B$ for fixed values of other control parameters such as $p$, $L_y$ etc.? Note that the limit $B = 0$ corresponds to a purely diffusive case, and a small positive value of $B$ will result in a faster walk in the $+x$ direction. As $B$ increases the motion should become faster (i.e., the gain in time should improve provided the temporary trapping of the particle in a dead end does not occur frequently). At the opposite extreme values of $B$ ($B \to 1$), on the contrary, the particle may become trapped for an extremely long time. At $B = 1$, even a very simple impurity cluster of the shape "$>$" in front of the particles' pathway will become absorbing; such an obstacle is liable to be encountered sooner or later if the sample is sufficiently large so that the probability that the particle never reaches the abscissa $l_x$ becomes nonzero. Therefore, at a fixed impurity concentration, there exists (at least) one value $B^*$ of $B$ which optimizes (i.e., minimizes) the first passage time of the particle at $l_x$. At low values of the impurity concentration $p$, $B^*$ is close to 1. As $p$ increases, $B^*$ decreases and $B^* \to 0$ as $p \to (1-p_c) \simeq 0.41$, i.e., when the concentration of the empty sites reaches its percolation threshold.

The existence of an optimum value $B^*$ of the bias in order to obtain the fastest traveling front of the particle through the sample has some practical interest (i.e., extraction of oil droplets through a porous medium) and, to our knowledge, has never been accounted for previously by a simple local mechanism. The main features of this observation are still valid in the case where there are many particles (or even, possibly, a constant feeding by the source in order to replace the departing particles, although in this case, collective pinning of the particles may obscure the observation). The same arguments can be extended to the mean front progression which reaches its maximum speed for some optimum value of $B$ as is qualitatively observed in our simulations. For example, $k \simeq 0.50$ at $B = 0.25$, $k \simeq 0.65$ at $B = 0.35$, $k = 0$ at $B = 0.50$. A precise evaluation of $B^*$ at each impurity concentration requires an enormous amount of computer time which is out of reach at present. Furthermore, our data indicate a deviation from the power-law dependence in a certain range of $B$ and $p$ (as we have seen above) where the value of $k$ may be meaningful only for the leading term in the variation of $R_f$ with $t$. Therefore, it is

rather difficult to comment more quantitatively on the characteristic value of $B$, beyond the qualitative level.

A similar analysis for the rms displacement of the particles and that of their center of mass is presented in Fig. 2; the $x$ and $y$ components are shown separately in Figs. 2(a) and 2(b), respectively. One might have expected that the forward bias would affect only the $x$ component of the rms displacement; however, we observe that both the $x$ and $y$ components of the motion are affected by the biased field. At $B_{+x} = 0.35, p = 0.30$, we find a very good power-law dependence of the $x$ component of the rms displacement of particles, $R_{tr}(x)$, and that of their center of mass, $R_{c.m.}(x)$ on $t$; the exponent $k'$ for both $R_{tr}(x)$ and $R_{c.m.}(x)$ in the asymptotic regime turns out to be about 0.60 [see Fig. 2(a)]. The magnitude of the exponent $k'$ decreases on increasing the forward bias (i.e., at $B_{+x} = 0.40$, $k' = 0.38$ and $k'$ vanishes at $B_{+x} = 0.50$). Note that the asymptotic exponent $k'$ for each particle on average and for their collective transport is smaller than that of the mean wetting front for the motion along the $+x$ direction. This means that the wetting (or fluid) front which is the locus of the first-passage front is followed by its carriers. An obvious part of this statement consists in the observation that the center of mass of
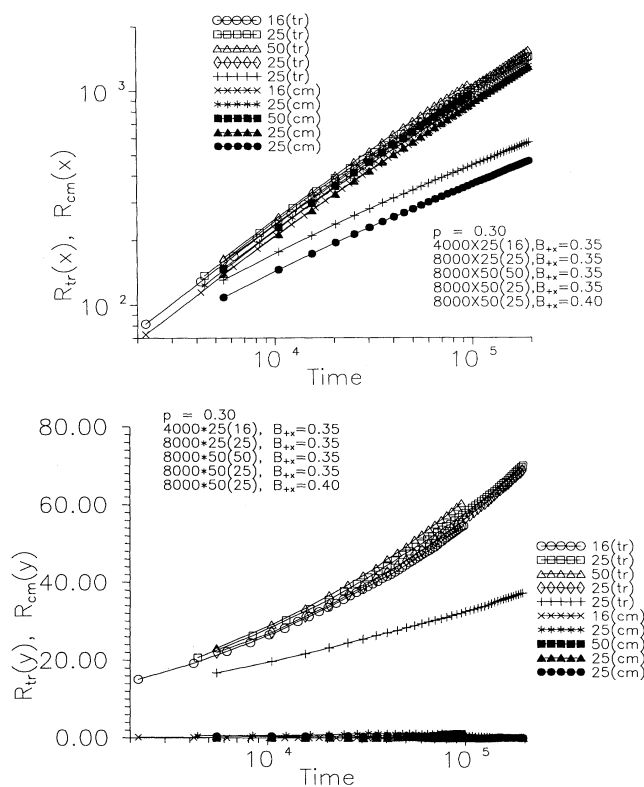


FIG. 2. (a) $X$ component of the rms displacement of the particles $R_{tr}(X)$ and that of their center of mass $R_{c.m.}(X)$ vs time on a log-log plot. The numbers on the rightmost side are the values of the forward bias $B_{+x}$. The same statistics is used as in Fig. 1. (b) Similar plot as (a) for the $y$ components of the rms displacements on a semilog scale.

tracers is located, as it should be, behind the mean wetting front location. However, a less trivial effect is displayed by the fact that the ratio of these quantities, say $R_{fx}/R_{trx}$, behaves as $t^{k-k'}$ with $k-k' \simeq 0.03$ at $B_{+x}=0.40$, and should therefore go very slowly to infinity as $t$ goes to infinity. We have not been able to confirm this tendency because of the enormous CPU time required. Even if this effect is transient and if $R_{fx}/R_{trx}$ should go to a constant value, the significance of the wetting process involved is clear. It means that the wetting front is created mainly by extreme and infrequent incursions of tracers which promptly return to their mean location area afterward.

The $y$ component of the center of mass of the particles seems to remain stable around zero [Fig. 2(b)]. The $y$ component of the rms displacement of each particle, $R_{tr}(y)$, on the other hand shows a systematic increase with time. At $B_{+x}=0.35$, $R_{tr}(y) \sim t^{k''}$ with $k''$ around $\frac{1}{3}$ while at $B_{+x}=0.40$, $k''$ is about $\frac{1}{5}$. The concentration of the allowed sites for the particles' motion is $1-p=0.70$ which is above the site percolation threshold (0.592). We know [1] that the random-walk motion of a single particle is diffusive (with $k''=\frac{1}{2}$) above the percolation threshold and anomalous (with $k''=\frac{1}{3}$) at the percolation threshold. Since there is no biased field along the $y$ direction, one would have expected a diffusive behavior for the $y$ component of the tracers' rms displacement $R_{tr}(y)$. Our data suggest a different type of driven diffusive transport behavior along the $y$ direction. Lower estimates of $k''$ at higher values of $B_{+x}$ indicate that the bias field affects the motion of the particles which become correlated in this model.

We have also studied the growth of the interface width $W$ (which is nothing but the mean wall thickness), $W^2 = \langle R_f^2 \rangle - \langle R_f \rangle^2$. A typical variation of $W$ versus $t$ on a log-log scale is shown in Fig. 3 for various sets of $N_p$ at $p=0.30$, and $B_{+x}=0.35$ and 0.40. The width grows with time and finally saturates (see Fig. 3). In fact the time evolution of $W$ clearly shows an overshooting before
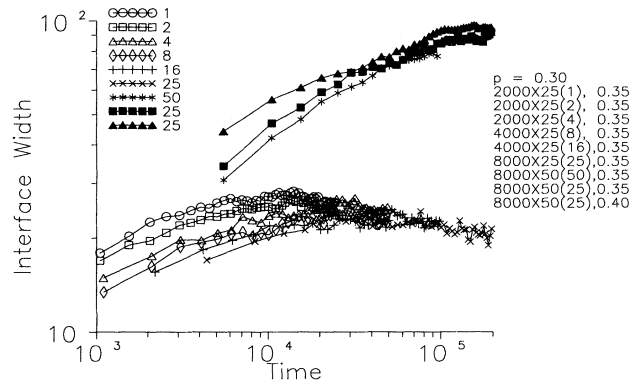


FIG. 3. Interface width vs time on a log-log scale with the same statistics as in Fig. 1. The rightmost numbers are the values of biased field in the $+x$ direction.

the saturation is reached. However, this saturation value $W_s$ is hard to evaluate with good accuracy due to its slow approach in the long-time regime. We note that the saturation width $W$ seems independent of the number of carriers. The difference in saturation width for different transverse lengths $L_y$ is evident; the lower curves are with $L_y=25$ while the upper curves correspond to $L_y=50$. Whether the wall thickness does indeed go to infinity as $L_y$ goes to infinity is yet to be proved. Even if we assume the size scaling $W_s \sim L_y^{\alpha}$, an estimate of $\alpha$, given the comparatively small number of sample widths used in this study, seems out of reach at present.

[1] R. B. Pandey, Phys. Rev. A 30, 489 (1984).
[2] S. F. Edwards and D. R. Wilkinson, Proc. R. Soc. London Ser. A 381, 17 (1982).
[3] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. 56, 889 (1986).
[4] D. Stauffer and J. G. Zabolitzky, Phys. Rev. Lett. 57, 1809 (1986); D. E. Wolf and J. Kertesz, Eur. Phys. Lett. 4, 651 (1987); P. Devillard and H. E. Stanley, Physica A 160, 298 (1989).
[5] F. Family, Physica A 168, 561 (1990); P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, Phys. Rev. A 34, 5091 (1986); D. Liu and M. Plischke, Phys. Rev. B 38, 4781 (1988); J. M. Kim and J. M. Kosterlitz, Phys. Rev. Lett. 62, 2289 (1989).
[6] Dynamics of Fractal Surfaces, edited by F. Family and T. Vicsek (World Scientific, Singapore, 1991).
[7] S. V. Buldyrev, A.-L. Barabasi, C. Caserta, S. Havlin, H. E. Stanley, and T. Vicsek, Phys. Rev. A 45, R8313 (1992).
[8] A.-L. Barabasi, M. Araujo, and H. E. Stanley, Phys. Rev. Lett. 68, 3729 (1992).
[9] J. Krug and H. Spohn, Phys. Rev. Lett. 64, 2332 (1990).
[10] H. G. E. Hentschel and F. Family, Phys. Rev. Lett. 66, 2348 (1991).
[11] Z.-W. Lai and S. Das Sarma, Phys. Rev. Lett. 69, 3195 (1991).
[12] H. Yan, Phys. Rev. Lett. 68, 3048 (1990).
[13] E. Willett and R. B. Pandey, Phys. Rev. Lett. 65, 3413 (1990).
[14] F. Family and R. B. Pandey, J. Phys. A 25, L745 (1992).
[15] M. A. Rubio, C. A. Edwards, A. Dougherty, and J. P. Gollub, Phys. Rev. Lett. 63, 1685 (1989).
[16] T. Nattermann, S. Stepanow, L.-H. Tang, and H. Leschhorn, J. Phys. II (France) 2, 1483 (1992).
[17] L.-H. Tang and H. Leschhorn, Phys. Rev. A 45, R8309 (1992).
[18] J. Koplik and H. Levine, Phys. Rev. B 32, 280 (1985).
[19] N. Martys, M. O. Robbins, and M. Cieplak, Phys. Rev. B 44, 12 294 (1991).
[20] R. B. Pandey (unpublished).