

# Universality in diffusion front growth dynamics

A. Hader, A. Memsouk, and Y. Boughaleb<sup>a</sup>

Laboratoire de Physique de la Matière Condensée, Université Hassan II- Mohammedia, Faculté des Sciences Ben M'sik, BP 7955, Casablanca, Morocco

Received 14 November 2001 / Received in final form 20 April 2002

Published online 31 July 2002 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2002

**Abstract.** We have studied the scaling properties of diffusion fronts by numerical calculations based on the mean field approach in the context of a lattice gas model, performed in a triangular lattice. We find that the height-height correlation function scales with time  $t$  and length  $l$  as  $C(l, t) \approx l^\alpha f(t/l^{\alpha/\beta})$  with  $\alpha = 0.62 \pm 0.01$  and  $\beta = 0.39 \pm 0.02$ . These exponent values are identical to those characterising the roughness of the diffusion fronts evolving through a square lattice [1,2], thus confirming their universality.

**PACS.** 05.50.+q Lattice theory and statistics (Ising, Potts, etc.) – 05.60.Cd Classical transport – 68.35.Fx Diffusion; interface formation

## 1 Introduction

The growth dynamics and formation of rough interfaces have received a lot of attention in recent years. Intense theoretical, numerical and experimental investigations have been developed within the subject in order to try understand the roughening process of fluctuating interfaces [3–9]. When the interfaces grow and roughen due to thermal fluctuations, the origin of the randomness arises due to the random nature of the deposition process (ballistic deposition, Eden model, aggregation etc.), and the dynamics are described by equations of the type introduced by Edwards-Wilkinson (EW) [10] or by Kardar-Parisi-Zhang (KPZ) [11]. For a certain class of interface growth, the interface moves in a disordered medium with a finite velocity under the influence of an external driving force (propagation of flame fronts, paper wetting, fluid flow in porous geometry...), the velocity of the interface is affected by the inhomogeneities of the medium, and the resistance of the medium to the flow results from a quenched disorder because it is frozen in time. The effects of the quenched randomness are modelled by the introduction of a time-independent term in the KPZ equation, which is the most general equation describing the motion of a driven interface in a disordered medium [12–14].

The dynamic scaling approach is an effective tool for characterising the temporal evolution of most interface phenomena and identifying the universality classes to which the different models belong. The most important quantities used to characterise the scaling of the interfaces is the global width parameter  $\omega(L, t)$  defined by,

$$\omega(L, t) = (\langle h^2 \rangle - \langle h \rangle^2)^{1/2} \quad (1)$$

where the function  $h(x, t)$  gives the height of the interface at time  $t$  and position  $x$ .  $L$  is the system size and  $\langle \rangle$  denotes a spatial average over the whole system. It has been shown [4] that the width of an interface scales with time  $t$  and system size  $L$  as,

$$\omega(L, t) \approx L^\alpha f(t/L^{\alpha/\beta}). \quad (2)$$

The function  $f(x)$  satisfies  $f(x \ll 1) \sim x^\beta$  and  $f(x \gg 1) \sim \text{const}$ . The exponents  $\alpha$  and  $\beta$  are called the roughness and growth exponents, respectively. The invariance property under the scale transformation implies that there is no characteristic length scale in the system besides the system size, and thus all scales obey the same physics. Hence, the scaling behavior of the interface can be obtained by measuring the local width over a window of size  $l \ll L$  at the interface,

$$\omega(l, t) \sim \begin{cases} t^\beta & \text{if } t \ll t_c(l) \\ l^\alpha & \text{if } t \gg t_c(l) \end{cases} \quad (3)$$

where  $t_c(l) = l^{\alpha/\beta}$ .

This study is a complementary of to our preceding work [1,2], in which we have investigated the scaling properties of non-equilibrium one-dimensional interfaces, called diffusion fronts, which diffuse through an inhomogeneous system, of square lattice geometry. The non-interacting and interacting cases have been treated. Here we simulate the growth dynamics of the diffusion fronts propagating in a triangular lattice in order to verify the universality of the scaling exponents describing the roughening kinetic of these interfaces. The calculations are performed using the mean field master equation within the framework of a lattice gas model, and the results are analysed with a dynamic scaling approach.

<sup>a</sup> e-mail: yboughaleb@yahoo.fr

## 2 Lattice gas model: mean field approach

The space is subdivided on cells represented by sites constructing a lattice. The sites can be occupied or empty. For each site  $i$ , we define an occupation number  $n_i$  which takes the value 0 or 1 to designate respectively, an empty or a full site. The set of all the occupation numbers at a given moment is called a configuration. For a lattice of  $N$  sites labelled by their coordinates  $i = 1, 2, \dots, N$ ; the configuration of particles can be written,

$$\{n\} = \{n_1, n_2, \dots, n_N\}. \quad (4)$$

When the particles interact, their Hamiltonian is given by,

$$H = - \sum_{i>j} \varepsilon_{ij} n_i n_j - \mu_0 \sum_i n_i. \quad (5)$$

For a repulsive interaction,  $\varepsilon_{ij} = \varepsilon < 0$  and  $\{i, j\}$  are nearest neighbour sites;  $\mu_0$  is the external chemical potential.

The diffusion process of the particles is insured by the change of the occupation numbers of the lattice sites. In the lattice gas formulation, this can be seen as the change of the lattice configuration. Then the dynamics of the lattice is governed by the phenomenological master equation which describes the evolution in time of the probability  $P(\{n\}, t)$ , having the configuration  $\{n\}$  at time  $t$ .

$$\frac{\partial(P\{n\}, t)}{\partial t} = \sum_{\{n'\}} \left[ \omega(\{n'\}, \{n\}) P(\{n'\}, t) - \omega(\{n\}, \{n'\}) P(\{n\}, t) \right]. \quad (6)$$

The rate of the configuration exchange is intended by the transition frequency  $\omega(\{n'\}, \{n\})$  which encodes all physical information about the considered system. The transition frequency is intended to satisfy the detailed balance condition that ensures the equivalence of transitions between the system's equilibrium states,

$$P_{eq}(\{n\}) \omega(\{n\}, \{n'\}) = P_{eq}(\{n'\}) \omega(\{n'\}, \{n\}). \quad (7)$$

The choice of an analytical expression for the transition frequency is obtained from the reference [9]. In our case, we restrict the jumps of the mobile particles between nearest neighbour sites only. Hence the transition frequency has the same form as in reference [1].

The average concentration over all possible configurations is defined by,

$$p(k) = \langle n_k \rangle = \sum_{\{n\}} n_k P(\{n\}, t). \quad (8)$$

The kinetic evolution is governed by the general master equation [16],

$$\frac{\partial p_k}{\partial t} \equiv \frac{\partial}{\partial t} \langle n_k \rangle = \sum_j \langle \omega_{jk}(\{n\}) n_j (1 - n_k) - \omega_{kj}(\{n\}) n_k (1 - n_j) \rangle. \quad (9)$$

The product  $n_j(1 - n_k)$  imposes the restriction that the site  $j$  is filled while the site  $k$  is empty.  $\omega_{kj}(\{n\})$  is the jump probability from site  $k$  to site  $j$ , depending on the local configuration. We restrict the jumps to those between nearest neighbour sites  $k$  and  $k + a$ . Hence, it is convenient to introduce a current operator  $J_{k, k+a}(\{n\})$  along the bond  $k \rightarrow k + a$ . Equation (6) then becomes,

$$\frac{\partial p_k}{\partial t} = - \sum_a \langle J_{k, k+a}(\{n\}) \rangle \quad (10)$$

(we have taken  $j = k + a$  in Eq. (6)).

The average current in the bond  $(i, j)$  is,

$$\langle J_{ij}(\{n\}) \rangle \equiv \langle \omega_{ij}(\{n\}) n_i (1 - n_j) - \omega_{ji}(\{n\}) n_j (1 - n_i) \rangle. \quad (11)$$

The model is a hopping model in which the jumps are between nearest-neighbour sites. The barrier that the particles have to overcome before making a jump, only depends on the depth of the initial site: the saddle point energy is insensitive to the environment and the energy of the final site has no influence on the jump probability. As the thermal energy is supposed small compared with the barrier heights, the jump probability follows an Arrhenius law. This leads to,

$$\omega_{ij}(\{n\}) = \omega_o \exp \left( - \frac{\varepsilon}{k_B T} \sum_{a \neq j-i} n_{i+a} \right). \quad (12)$$

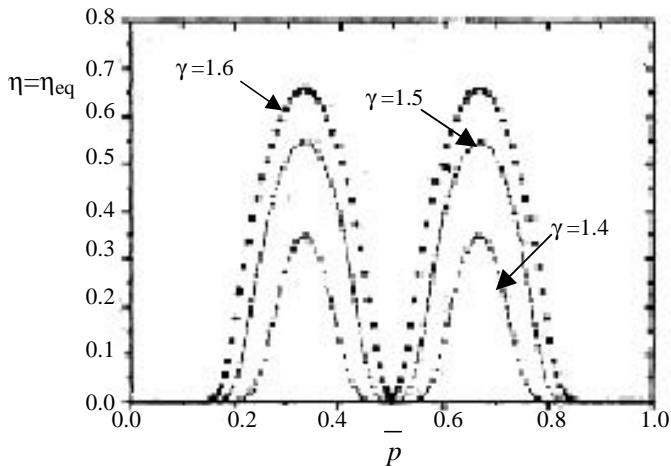
For systems with a repulsive nearest-neighbour interaction, the use of the lattice gas model is able to reproduce the order-disorder transition characterised by the break of the occupation symmetry of the lattice. Hence, we have to distinguish between various sublattices. The triangular lattice is supposed to be divided into three interpenetrating sublattices  $A$ ,  $B$  and  $C$  in the way that any site, say  $A$ , would have three nearest neighbours in each of the two other sublattices  $B$  and  $C$ . The average concentration evolution with respect to time, of each sublattice, satisfies equation (10). Then, we obtain three kinetic coupled equations,

$$\frac{\partial p^\alpha}{\partial t} = - \sum_a \sum_{\lambda \neq \alpha} \langle J_a^{\alpha\lambda}(\{n\}) \rangle \quad (13)$$

with  $\alpha, \lambda = A, B$  or  $C$  and  $\alpha \neq \lambda$ .

$$J_a^{\alpha\lambda}(\{n\}) \equiv \omega^{\alpha\lambda}(k, a) n_k^\alpha (1 - n_{k+a}^\lambda) - \omega^{\lambda\alpha}(k + a, -a) n_{k+a}^\lambda (1 - n_k^\alpha). \quad (14)$$

The mean field approximation is the simplest method that allows a primary understanding of the studied phenomenon by providing exact mathematical solutions although it can not completely describe the physical reality. In our case, the consideration of the mean field approach consists to replacing all the occupation numbers,  $n_k$ , by



**Fig. 1.** The parameter order *versus* mean concentration for different reduced energies.

their average concentration,  $p_k$ . Then, the general expression for the current in equation (13) for the mean field approach can be written,

$$J_a^{\alpha\lambda}(\{p\}) \equiv \langle \omega^{a\lambda}(k, a) \rangle p_k^\alpha (1 - p_{k+a}^\lambda) - \langle \omega^{\lambda\alpha}(k + a, -a) \rangle p_{k+a}^\lambda (1 - p_k^\alpha). \quad (15)$$

where:

$$\langle \omega^{a\lambda}(k, a) \rangle = \omega_o \exp \left( -\frac{\varepsilon}{k_B T} \sum_{a \neq j-i} p_{k+a}^\lambda \right) \quad (16)$$

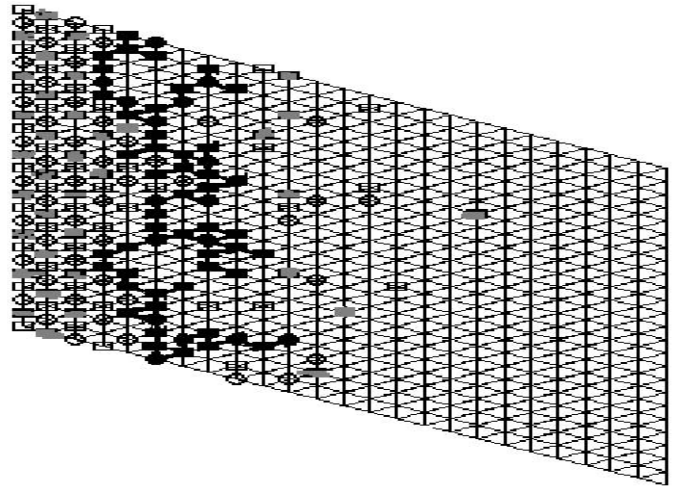
and  $\gamma = -\frac{\varepsilon}{k_B T}$  is the reduced interaction energy.

The numerical resolution of equation (13) in the presence of repulsive interactions shows an order-disorder transition for reduced interaction energies greater than a critical value,  $\gamma_c$ . The evaluation of the order in the system is done through the introduction of the order parameters  $\eta^{\alpha\lambda}$  which represent the difference between the occupancies of the three sublattices and are defined as follows:

$$\eta^{\alpha\lambda}(k) = |p^\alpha(k) - p^\lambda(k)| \quad (17)$$

with  $\alpha, \lambda = A, B$  or  $C$  and  $\alpha \neq \lambda$ .

The dependence of the order parameter on the lattice average concentration is represented for different values of the reduced energy in Figure 1 [17]. We notice that the order in the lattice is related to a break in the occupation symmetry of the lattice and that the order extension depends on the interaction regime. The order parameter  $\eta$  presents a maximum at the concentration  $1/3$  and  $2/3$  relative to the formation of the ordered phases. The long range order at  $p = 1/3$  corresponds to the filling of one sublattice while the two others sublattices are empty. For the concentration  $p = 2/3$  we have the opposite case [17]. More details on the dynamics of the order-disorder transition for the triangular lattice are given in references [17, 18].



**Fig. 2.** A qualitative picture of the diffusion on a triangular lattice. The bold line which joins the black points represents the diffusion front.

### 3 The scaling behaviour of the diffusion front

We perform the diffusion on a triangular lattice, semi-infinite in the  $x$  direction ( $x > 0$ ) and periodically bounded in the  $y$  direction. There is a source at the position  $x = 0$  ( $p(x = 0, \forall t) = 1$ ) which feeds the initial empty system and a well at a sufficiently large abscissa ( $p(x_M, \forall t) = 0$ ). We distribute the density profile solution of (13) in this case on a triangular lattice by associating, to each site of the lattice at random, a positive value less than one. The value is compared with the value of the concentration profile at the same abscissa obtained by solving equation (13). The result of the comparison defines the occupation state of the lattice sites: if the random number is less than the value of the concentration at the same site the latter will be occupied; otherwise the site remains empty.

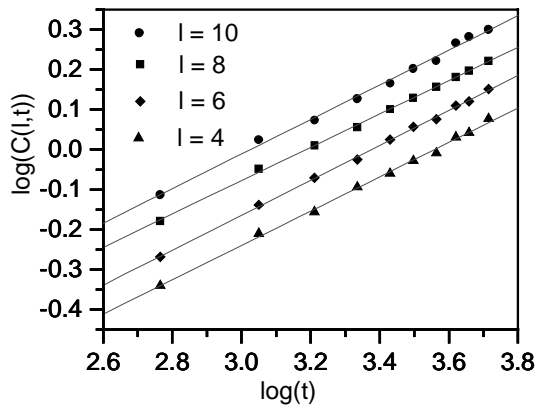
#### 3.1 The non-interacting case ( $\gamma = 0$ )

In this case, we have distributed the density profile solution of (13) under the above conditions. Figure 2 is a simulation of the diffusion process. The outermost line of particles still connected to the source is the diffusion front. It has been shown that the mentioned interface has a fractal aspect and can be identified as the hull of the percolation cluster.

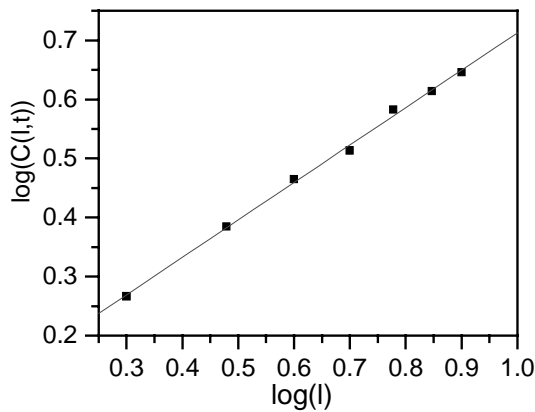
From a computational point of view, it is convenient to determine the scaling exponents describing the growth width of the diffusion front by using the height-height correlation function  $C(l, t)$ ,

$$C(l, t) = \left[ \langle h(i+l, t) - \bar{h}(i, t) \rangle_i^2 \right]^{1/2} \quad (18)$$

as it scales in the same way as the local width  $\omega_L(l, t)$  over a portion of length  $l$  on the interface ( $C(l, t) \approx \omega_L(l, t) \approx l^\alpha f(t/l^{\alpha/\beta})$ ). We define  $h(i, t)$  as the last particle in row  $i$



**Fig. 3.** The height-height correlation function *versus* time  $t$ , on a log-log plot in the non-interacting case and for different lengths  $l \ll L$ . the time  $t$  is shorter than the cross-over time  $t_c$ , where the width saturates.

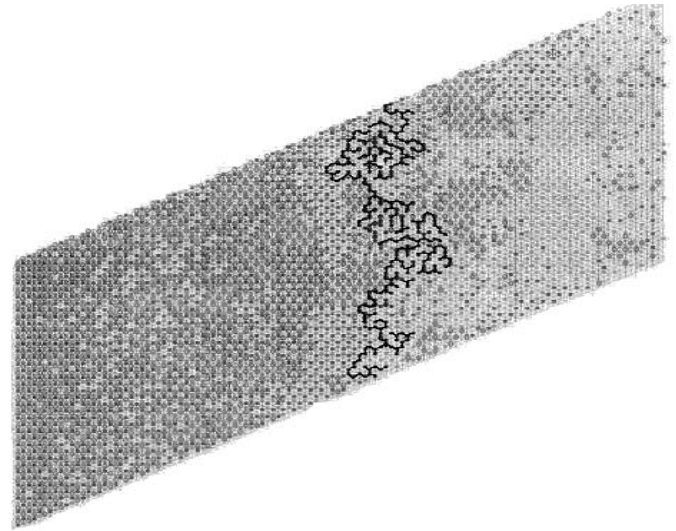


**Fig. 4.** The saturation height-height correlation function *versus* length  $l$  on log-log scales in the non-interacting case.

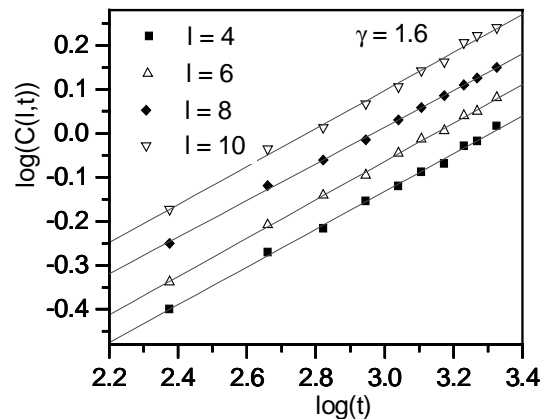
belonging to the front. The simulation results for a system of global width  $L = 50$  are reported in Figures 3 and 4. This leads to a growth exponent  $\beta = 0.39 \pm 0.02$  and a roughness exponent  $\alpha = 0.62 \pm 0.01$ , consistent with the critical exponents describing the roughening of fronts diffusing in a square lattice [1,2]. Then, the diffusion front scaling exponents are lattice- independent.

### 3.2 The repulsive interaction case ( $\gamma \neq 0$ ) and discussion

In order to check the effect of the interaction on the scaling behaviour of the diffusion front, we have introduced the repulsive interaction between nearest neighbour, sites susceptible to produce an order-disorder transition in the system. We distribute the density profile solution of (13), in this case, on a triangular lattice. Figure 5 is a simulation of the diffusion process in presence of an order-disorder transition. This picture shows a distribution of ordered domains in the lattice and the diffusion front can be seen as an interface which delimits the disordered and ordered region. We have also calculated the local width of the diffusion front and we have found that it scales with time

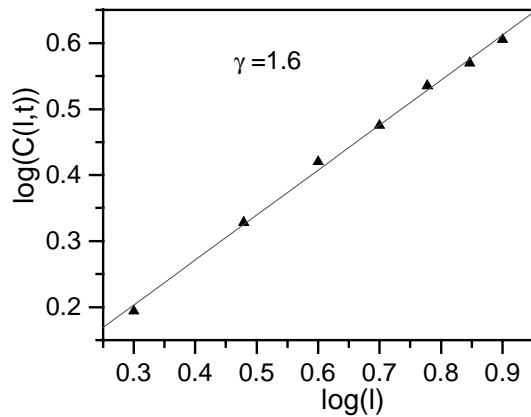


**Fig. 5.** A qualitative picture of the diffusion on a triangular lattice in the presence of an order-disorder transition at a given time  $t$ . The bold line which joins the black points represents the diffusion front.



**Fig. 6.** The height-height correlation function *versus* time  $t$ , on log-log scales for different lengths  $l \ll L$ , for an interaction value  $\gamma = 1.6$  and for times shorter than the cross-over time  $t_c$  where the width saturates.

$t$  and length  $l$  as  $C(l, t) \approx \omega_L(l, t) \approx l^\alpha f(t/l^{\alpha/\beta})$ , with  $\alpha = 0.62 \pm 0.02$  and  $\beta = 0.40 \pm 0.01$  (see Figs. 6 and 7). These exponent values are identical to those characterising the roughness of the diffusion fronts in the non-interacting case. Thus the scaling properties of the diffusion fronts are not affected by the interactions. This result was verified in the square lattice case [1]. The scaling exponent values are larger than those predicted by the (1+1) dimensional Edwards-Wilkinson and KPZ equations, and belong to the scaling picture developed by different experiments and simulations concerning driven interfaces in disordered media. Thus confirming our conjecture that our model is able to reproduce the scaling dynamic features of the invasion percolation fronts, and that the inhomogeneous disorder in our model, constituted by the finite ordering clusters in the vicinity of the diffusion front, has the same effect



**Fig. 7.** The saturation height-height correlation function *versus* length  $l$  on log-log scales for an interaction value  $\gamma = 1.6$ .

as the quenched disorder in generating exponents larger than those predicted by the theory [1]. Indeed our model possesses the same features as interfaces moving in disordered media; a driving force which can be expressed as a function of the local concentration gradient as  $F \sim 1/|\nabla p|$  – the diffusion front is located at a critical concentration  $p_c$  corresponding to a critical driving force  $F_c \sim 1/|\nabla p_c|$  ( $|\nabla p_c|$  denotes the concentration gradient at concentration  $p_c$  corresponding to the front position). The random distribution of ordered clusters just nearby the front is static and, in average, has the same effect as the quenched disorder on the other driven interfaces. Moreover, our model is appropriate to the experimental problem of injection of a fluid in a porous medium. The similarity between the fluid flow experiment and our model is well established in [1].

## 4 Conclusion

The important conclusion of this work is that we have verified the universality of the scaling exponents characterising diffusion front growth dynamics. After having shown in preceding works [1,2], that these exponents are not affected by the interactions, we have displayed here that neither do they not depend on the lattice geometry. The critical exponents  $\alpha$  and  $\beta$  describing the diffusion front scaling behaviour are larger than the EW and the KPZ exponents. We have explained this anomalous roughening by the presence of finite ordering clusters in the vicinity of the diffusion front. This constitutes an inhomogeneous

disorder that has the same effect as the quenched randomness present in interfaces moving in disordered media. All these arguments prove that the diffusion fronts can be integrated into the category of interfaces in disordered media.

The authors would like to thank Professor R. Nassif for his fruitful discussions.

## References

1. A. Memsouk, Y. Boughaleb, R. Nassif, H. Ennamiri, *Eur. Phys. J. B* **17**, 137 (2000)
2. A. Memsouk, Y. Boughaleb, R. Nassif, H. Ennamiri, M. J. *Cond. Matt.* **2**, 35 (2000)
3. J. Krug, H. Spohn, in: *Solids Far From Equilibrium: Growth, Morphology and Defects*, edited by C. Godrèche (Cambridge University Press, Cambridge, 1991)
4. A.L. Barabasi, H.E. Stanley, *Fractal Concept in Surface Growth* (Cambridge University Press, Cambridge, England, 1995)
5. T. Viscek, in *Fractal Growth Phenomena*, 2nd edn. (World Scientific Singapore, 1992)
6. F. Family, T. Viscek, *J. Phys. A* **18**, L 75 (1985)
7. J.M. Lopez, J. Schmittbuhl, *Phys. Rev. E* **57**, 6405 (1998); *Phys. Rev. E* **58**, 6999 (1998)
8. J.M. Lopez, H.J. Jensen, *Phys. Rev. Lett* **81**, 1734 (1998)
9. F. Family, K.C.B. Chan, J. Amar, *Dynamics of interface roughening in imbibition' in Surface Disordering: Growth, Roughening and Phase Transitions*, edited by R. Jullien, J. Kertesz, P. Meakin, D.E. Wolf (Nova Science, New York, 1992), pp. 205–212
10. S.F. Edwards, D.R. Wilkinson, *Proc. R. Soc. London A* **381** 17 (1982)
11. M. Kardar, G. Parisi, Y-C. Zhang, *Phys. Rev. Lett.* **56**, 889 (1986)
12. D.A. Kessler, H. Levine, Y. Tu, *Phys. Rev. A* **43**, 4551 (1991)
13. G. Parisi, *Europhys. Lett.* **17**, 673 (1992)
14. Z. Csahok, K. Honda, T. Vicsek, *J. Phys. A* **26**, L171 (1993)
15. J.F. Gouyet, *Phys. Rev. E* **51**, 1695 (1995)
16. R. Nassif, Y. Boughaleb, A. Hekkouri, J.F. Gouyet, M. Kolb, *Eur. Phys. J. B* **1**, 453 (1998)
17. H. Ennamiri, R. Nassif, Y. Boughaleb, J.F. Gouyet, *J. Phys. Cond. Matt.* **9**, 1 (1997)
18. H. Ennamiri, R. Nassif, Y. Boughaleb, *Phys. A* **238**, 252 (1997)