Diffusion limited propagation of burning fronts

Massimo Conti, Umberto Marini Bettolo Marconi
Dipartimento di Fisica, Universita' di Camerino, I-62032, Camerino, Italy
e-mail: massimo.conti@unicam.it

Abstract

In this numerical study we simulate flame propagation when the limiting transport mechanisms is the diffusion of oxygen and heat. This situation may be representative of smouldering combustion in the forest ground, when the intricate vegetation structure prevents the onset of large scale convection. The interplay between the diffusion processes results in a dynamical instability with a tendency of the burning front to develop cellular or dendritic patterns. The typical length scale associated with the observed patterns results to be a combination of the diffusion lengths associated with the two competing processes.
Keywords: flames propagation,pattern instability

1 Introduction

Flame propagation is a complex process involving chemical reactions and transport phenomena [**?**]. The advancing of the combustion front is sustained by the self-produced heat and is rate limited by the availability of both fuel and oxidant. In general, the transport phenomena in the environment where the burning front propagates involve both heat and oxygen convection. However, in the smoldering combustion of the forest ground, when the intricate

vegetation structure prevents the onset of large scale convection processes, diffusion may become the rate limiting mechanism. It is the situation observed in a variety of growth phenomena such as solidification processes, viscous fingering, electrochemical deposition, diffusion limited aggregation, dielectric breakdown [**?**]. In such phenomena the front of the growing phase is morphologically unstable and evolves into a complex pattern, with production of fingers, grooves, side-branches and dendritic structures. For many of these phenomena typical properties such as the velocity of the front and the length of the patterns can be related to well studied quantities such as surface tension, chemical potential differences, temperature gradients. This analogy stimulates interesting questions about the connection between the morphological instability of the burning front and the one related to dendritic growth in rapid solidification and similar phenomena.

As shown in the classical work of Mullins and Sekerka, [**?**], the morphological instability observed in diffusion controlled growth arises as the growth process requires transportation of some conserved quantity away or towards the growing interface, and the fragmentation of the advancing front into a large surface area favors the diffusion processes. On the other side a large interface area is too costly in terms of surface energy, and the competition of these two effects determines the dynamics of the process and the characteristics of the interface pattern. Is this mechanism useful to give some insight into the flame propagation problem? Is some factor playing the role of surface tension in this problem? We shall answer these questions starting from a simple lattice model [**?**] in which two diffusive fields, and a reactive field proposed on a purely phenomenological basis, interact and give rise to a rich variety of patterns.

The paper was stimulated by experimental studies performed by Zik, Olami and Moses [**?**, **?**] with a two-dimensional apparatus. These researchers used a thin rectangular chamber to study the combustion of a paper sheet. The thin gap between the two plates prevented convection transport of heat and oxygen. Measurements were made when the combustion was very slow -that is, the fuel was smoldering, a non flaming mode in which the emitted gas doesn't glow. In these conditions a fingering instability was observed.

The paper is organized as follows: in section 2 we introduce and motivate the model, in section 3 we present the results of the simulations of the lattice model for various choices of the control parameters, in section 4 we draw the conclusions.

2 A minimal model for combustion propagation

The propagation of a burning front is a complex phenomenon which involves several heterogeneous reactions. Details of the reactions kinetics are poorly understood, but some aspects of the global picture can be captured by a minimal model which refers to only a limited number of dynamic variables. In particular, the interfacial instabilities of the burning fronts observed in some experiments in two dimensions can be predicted and interpreted.

At a basic level of description, the combustion advances through the solid fuel in a competition between endothermic pyrolysis and exothermic oxidation. Then, the dynamics of the process is characterized only by three fields: the oxygen, the fuel and the heat released by the reaction.

The fuel can react with oxygen, in a local irreversible transformation from an unstable state before ignition towards a final stable state. On the other hand, oxygen and heat are transported by diffusion processes towards and away from the advancing front, respectively.

In the model we propose the three fields are defined on a discrete two dimensional square lattice, where each location is labeled by i. Then, three dynamical variables A_i,C_i and H_i represent the oxygen concentration (A_i),the combustible C_i, which takes on the values 0 or 1 in the unburned or burned state respectively, and the heat amount H_i.

The dynamics of the three variables is developed along a discrete time grid, according to the following evolution rules:

1) a site i is chosen randomly .

2) if both the local heat and oxygen variables H_i and A_i are above some fixed thresholds (S_H and S_A) the discrete variable C_i will change its state ($0 \to 1$) in an irreversible fashion, representing the combustion of the site.

3) Due to combustion the site releases a certain amount of heat and consumes oxygen according to the following scheme:

$$C_i' = C_i + 1$$

$$H_i' = H_i + \Delta H$$

$$A_i' = A_i - \Delta A$$

4) The oxygen molecules diffuse towards the reaction zone, while the heat diffuses away from there. The two processes occur at different rates.

This model is inspired to our earlier work [**?**], where solidification processes in binary alloys were described through a microscopic dynamics with

stochastic character. In that case the process was reduced to a diffusion-reaction dynamics with two diffusive fields (temperature and solute concentration), recovering the observed macroscopic behavior at a microscopic and mesoscopic scale without coarse graining the model. However a main differences with respect to the solidification problem is that the combustion reaction is an irreversible process with no analogue in the solidification problem, where the material field may undergo either the liquid to solid transformation or the reverse.

Moreover,combustion has no analogue to the surface energy cost between neighboring sites belonging to different states, lacking a mechanism for the morphological stabilization of the burning front. The latter point raises the question whether some other factor plays the same role. To this regard we observe that the ignition at a site i is activated only if a sufficient amount of thermal energy (heat) is present. Heat is released by combustion of nearest burned sites,but is dispersed away by diffusion towards colder regions. However, if the associated thermal diffusion length is sufficiently short the result will be that of a stabilizing force similar to a surface tension, because only sites close to a site which is releasing heat can light up. On the other side the oxygen required for combustion at a given site must be transported there by diffusion. Thus the need for fresh oxygen tends to favor the formation of a large interface area. The balance between these two competing forces leads to a dynamical instability of the propagation front between the burned and unburned material, whose characteristics will change according to the experimental conditions.

3 Numerical Results

We performed simulation runs of the reactive-diffusive model described above in the xy plane, using a 512×512 lattice. In the initial configuration the sites are unburned ($C = 0$) and cold ($H = 0$), and the oxygen concentration is uniform ($A = A_0$). To start the combustion a thin strip ($x < x_0$) at the left border of the domain is prepared in the "hot" state ($H = 1$). In our simulations we fixed the oxygen concentration threshold at $S_A = 1$; the release of heat and the oxygen consumption are assumed to be $\Delta H = \Delta A = 1$. The combustion process was followed up to N Montecarlo steps (MCS), until a well defined regime was attained. The diffusion mechanism for the heat and oxygen fields was simulated via a random exchange between a site and its nearest neighbors; the two different diffusive time scales were controlled by iterating independently, for each MCS, the related attempts of exchange. The resulting frequencies of attempt (per MCS) will

be indicated in the following as f_H and f_O, respectively. To present the numerical results all lengths will be measured in lattice spacing units and the non-dimensional time will be expressed in MCS.

The structures developed in the combustion process strongly depend on the diffusion rate of the oxygen field.

In Figure 1 we show, at $t = 16000$, the cellular pattern which arises fixing $f_H = 0.2$, the oxygen concentration at $A_0 = 0.90$ and the heat threshold at $S_H = 0.50$. The frequency of attempt f_O (that means the diffusivity of the oxygen field) is set at $f_O = 1$.

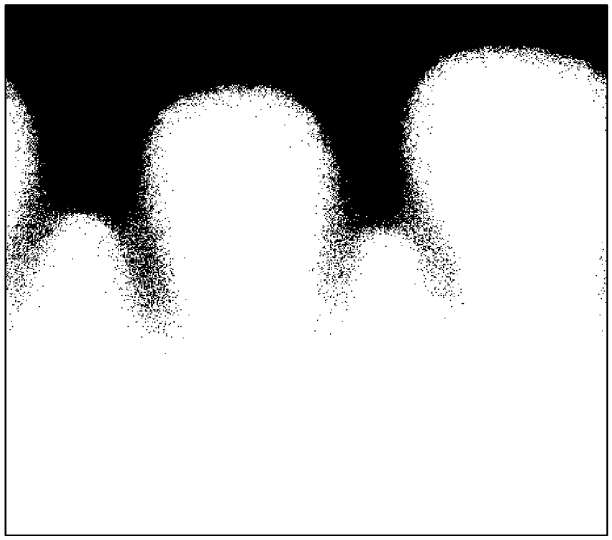

Figure 1: The combustion field at $t = 16000$ MCS.The initial oxygen concentration is $A_0 = 0.90$,the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 1$ respectively, the heat threshold is $S_H = 0.50$.

Similar structures are observed in the directional solidification of binary alloys beyond the onset of the Mullins-Sekerka instability. The characteristic length of the pattern is most usually selected through the competition of the stabilizing effect of the surface tension and the necessity to develop a large interface area to reject (or to draw) a conserved quantity. Both these phenomena can be described through natural length scales (the capillary length d_0 and the diffusion length l_d, respectively), and the wavelength of

the pattern emerges as $\lambda \sim \sqrt{d_0 l_d}$. Our model does not account for an interface energy cost, nevertheless a stabilizing effect, mimicking the role of surface tension, is still present, as the ignition is prevented when the local heat field is below the threshold S_H. But the heat released at a burning site is dissipated through a diffusion mechanism, in such a way that too fragmented structures are disfavoured.

According to the above considerations, we expect a thinner morphology of the combustion pattern with decreasing either the threshold S_H or the oxygen diffusion length L_O (that means decreasing the frequency of attempt f_O). This is the situation depicted in Figures 2 and 3. In Figure 2 ($f_O = 0.2$)we observe that the wavelength of the pattern has been strongly decreased, as we here observe five well developed cells of the burned fuel. In Figure 3 ($f_O = 1$, $S_H = 0.40$)the situation is even more clear, as we observe tip splitting and a side-branch activity that indicates that the pattern is driven towards a dendritic regime.

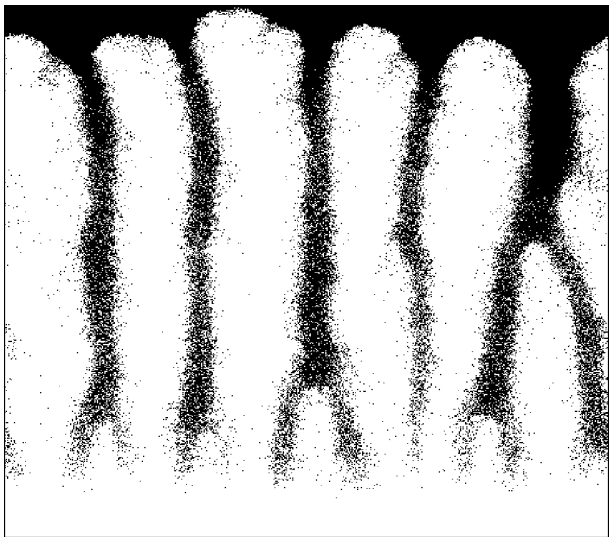

Figure 2: The combustion field at $t = 16000$ MCS.The initial oxygen concentration is $A_0 = 0.90$,the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 0.2$ respectively, the heat threshold is $S_H = 0.50$.

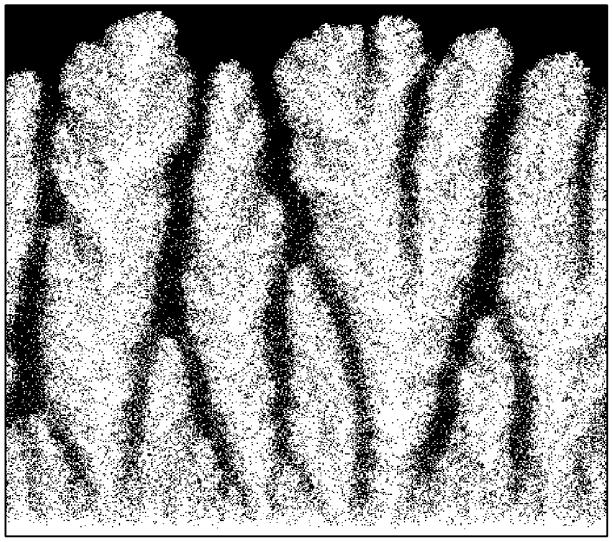

Figure 3: The combustion field at $t = 16000$ MCS.The initial oxygen concentration is $A_0 = 0.90$,the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 1$ respectively, the heat threshold is $S_H = 0.40$.

Notice that the concentration of oxygen is initially fixed at a value below the threshold S_A, and to sustain the combustion oxygen must be drawn towards the interface. Then, a compact front would be slowed down with the growth rate decaying as $t^{-1/2}$. But a cellular or dendritic structure can develop at constant growth rate if the burnt sites left behind the advancing front cover an area fraction equal to the initial oxygen concentration. This is precisely the situation shown in Figure 4, where the "mass" of the combusted sites is represented versus time.

The straight line (curve a) refers to the cellular growth addressed in Figure 2: we can observe that the combustion front advances at constant growth rate. For comparison we also show a curve (b) representative of compact growth conditions obtained with $f_O = 1, S_H = 0.45, A_0 = 0.60$. In the latter case we observe a typical diffusion-limited behavior, with the combustion front advancing as $\sim t^{\alpha}$: the deviation of the best fit value $\alpha = 0.53$ from the pure diffusional value $\alpha = 0.5$ can be attributed to a residual porosity of the combusted phase.

We observed that the morphology of the combusted phase is strongly

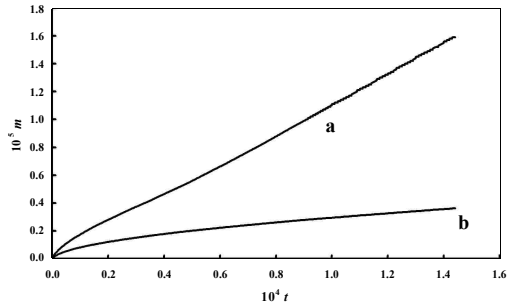

Figure 4: The mass of the combusted sites represented versus time. Curves a and b refer to cellular and compact growth, respectively

affected by the length scale of the oxygen field. The latter in turn depends on the frequency of attempts f_O, which is the microscopic counterpart of the macroscopic diffusion coefficient D. To elucidate this point we show in Figure 5 the oxygen concentration along the growth direction, at $t = 8000$. The two curves refer to the same sets of data employed in Fig. 1,2, and the oxygen field is averaged over the direction normal to the combustion propagation. We note that the width of the transition zone from the low concentration area (behind the combustion front) to the high concentration sites increases with increasing the oxygen diffusivity f_O.

Figure 6 shows the diffusion length L_O of the oxygen field versus f_O. The two curves refer (from top to down) to $S_H = 0.4$ and $S_H = 0.3$. L_O has been estimated as the length required for the transition from 20% to 90% of the concentration at infinity. Notice that a larger value of S_H reflects on a lower velocity of the process, and we recover the well known result that the diffusion length diminishes as the growth rate increases.

The above considerations suggest that a morphological phase diagram could be drawn in a S_H, f_O plane, where regions characterized by a large growth rate or low oxygen diffusivity should correspond to dendritic growth, whereas cellular patterns are likely to be found at large values of S_H and f_O. This kind of diagram is shown in Figure 7, for an initial oxygen concentration $A_0 = 0.75$.

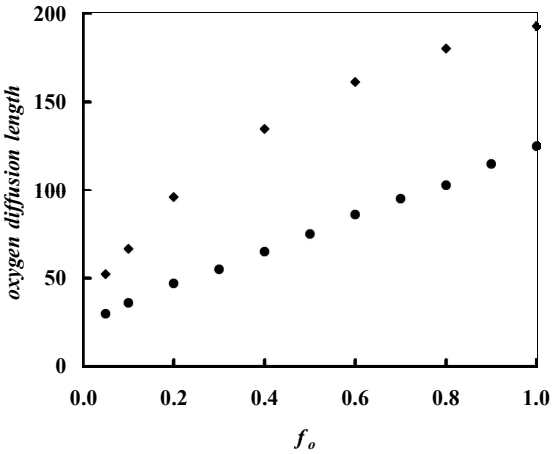

Figure 5: The profile of the oxygen field for the cellular growth shown in fig.1 (curve b) and in fig.2 (curve a)

4 Conclusions

In the present paper we have discussed a new lattice model which describes the formation and the advancing of a combustion front in the absence of convection. With respect to existing approaches to the problem we assumed a microscopic point of view, in the sense that we have not assumed from the start a coarse grained differential equation. Instead we have assumed the following set of stochastic evolution rules for the microscopic variables A_i,H_i,C_i representing respectively the local values of the oxygen, the heat and the combustible: a) a local rule for the C_i variable b) two diffusive rules for A_i and C_i plus source and sink terms respectively. The numerical simulations carried out in two dimensions at various diffusion rates display the trapping phenomenon of unburned combustible, and a complex morphology of the interfacial patterns which has allowed us to construct a phase diagram of the phenomenon.

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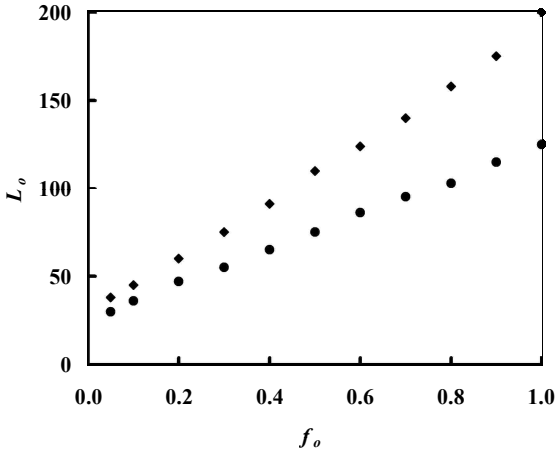

Figure 6: The diffusion length of the oxygen field versus the frequency of attempts f_O. The two curves were obtained with $S_H = 0.4$ (diamonds) and $S_H = 0.3$ (circles)

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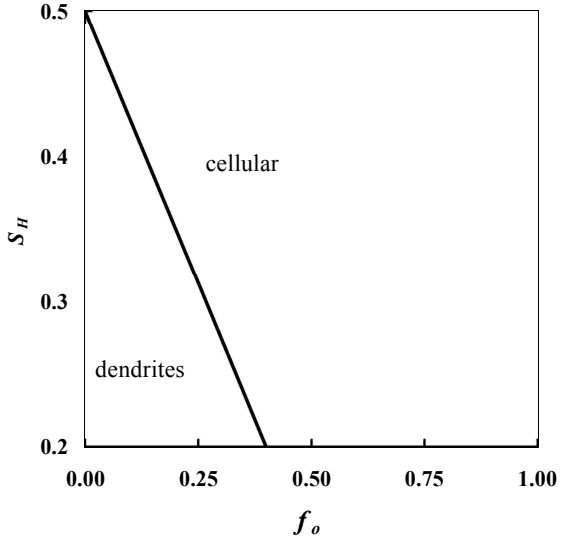

Figure 7: The morphological phase diagram for the pattern of the combustion field in the S_H, f_O plane.