

Diffusion limited propagation of burning fronts

M. Conti & U. M. B. Marconi

Dipartimento di Fisica, Università di Camerino, Italy

Abstract

In this numerical study we simulate burning 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 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 [1]. 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. Diffusion limited growth is the situation observed in a variety of growth phenomena such as solidification processes, viscous fingering, electrochemical deposition, diffusion limited aggregation, dielectric breakdown [2]. 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 [3], 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 combustion propagation problem? Is some factor playing the role of surface tension in this problem? We shall answer these questions using a simple lattice model [4] 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 et al. [5, 6] 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 does not 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 reacts with oxygen and releases heat, 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 ($0 \rightarrow 1$) 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. The diffusion mechanism is included by assuming that at every time step random exchange events take place between the nearest neighbors sites i and j in the lattice, so that for each event the post-collision conserved field E (E stays for heat or oxygen) is determined according to the rule $E'_i \rightarrow (E_i + E_j)r$ and $E'_j \rightarrow (E_i + E_j)(1 - r)$ where r is a random number chosen from a uniform distribution in the unit interval. By sweeping randomly the lattice the system behaves ergodically and one can compute meaningful statistical averages.

This model is inspired to our earlier work [7], 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 combustion front, 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 two diffusive time scales for the heat and oxygen fields 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 $A_O = 0.90$ and

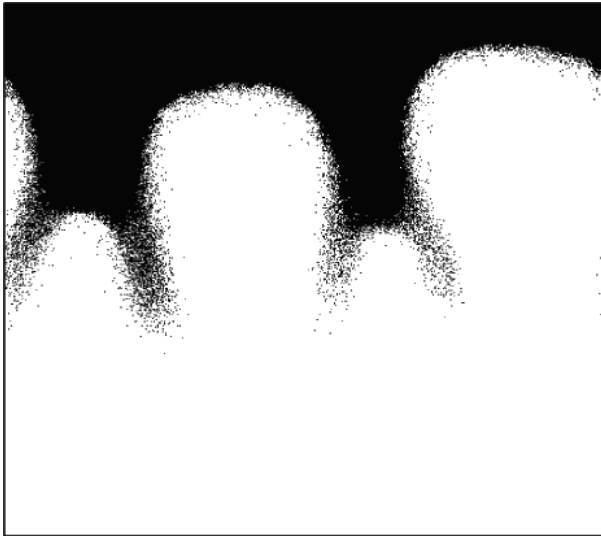


Figure 1: The combustion field at $t = 16000$ MCS. The initial oxygen concentration is $A_0 = 0.90$, the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 1$ respectively, the heat threshold is $S_H = 0.50$.

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 $f_O = 1$. 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 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 ($f_O = 0.2$, $S_H = 0.40$) 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.

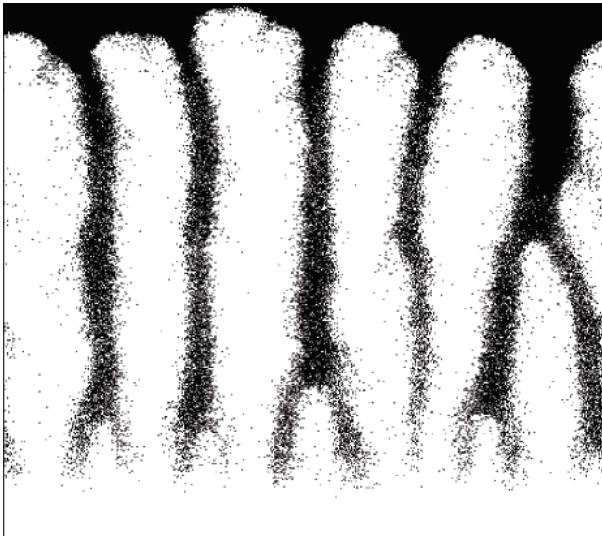


Figure 2: The combustion field at $t = 16000$ MCS. The initial oxygen concentration is $A_0 = 0.90$, the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 0.2$ respectively, the heat threshold is $S_H = 0.50$

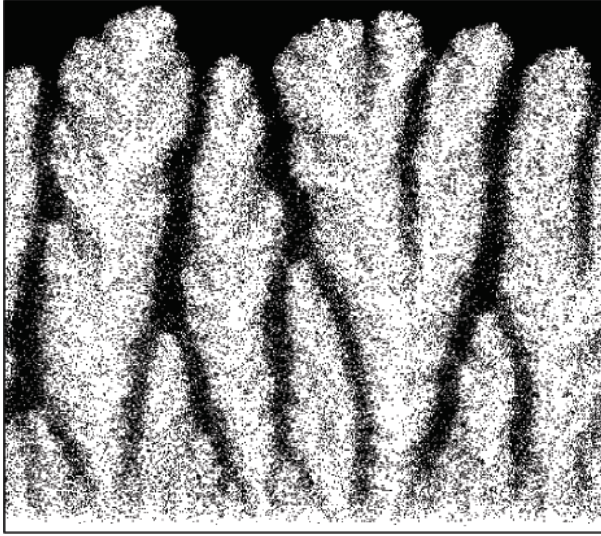


Figure 3: The combustion field at $t = 16000$ MCS. The initial oxygen concentration is $A_0 = 0.90$, the frequencies of attempt for the heat and the oxygen fields are $f_H = 0.2$ and $f_O = 0.2$ respectively, the heat threshold is $S_H = 0.40$.

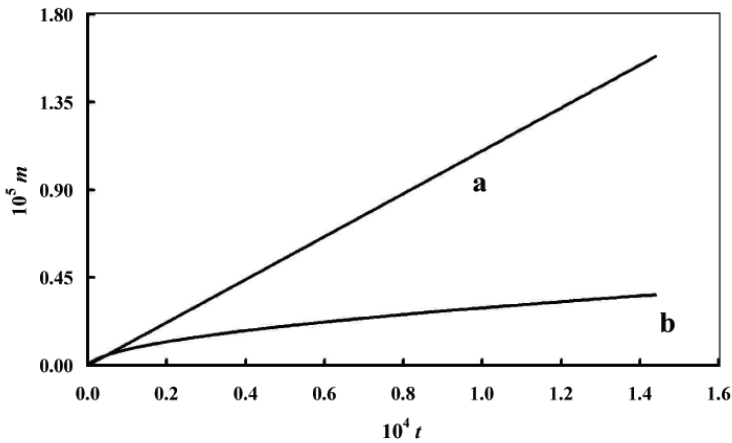


Figure 4: The mass of the combusted sites represented versus time. Curves a and b refer to cellular and compact growth, respectively.

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

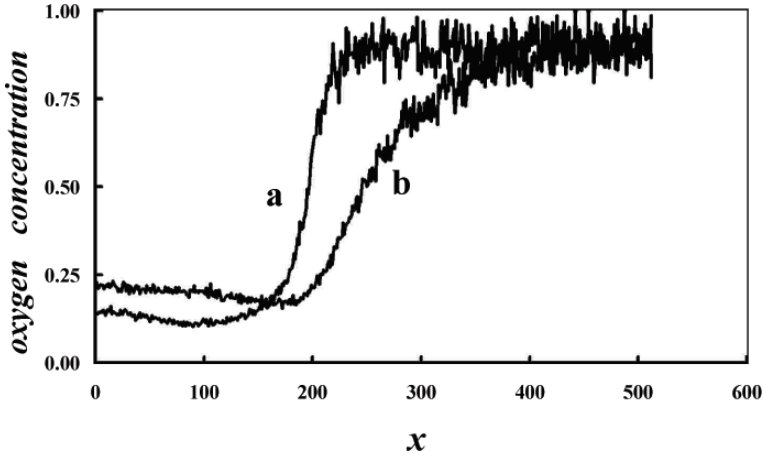


Figure 5: The profile of the oxygen field for the cellular growth shown in fig.1 (curve b) and in fig.2 (curve a).

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 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 Figs. 1 and 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 $S_H = 0.5$ 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.

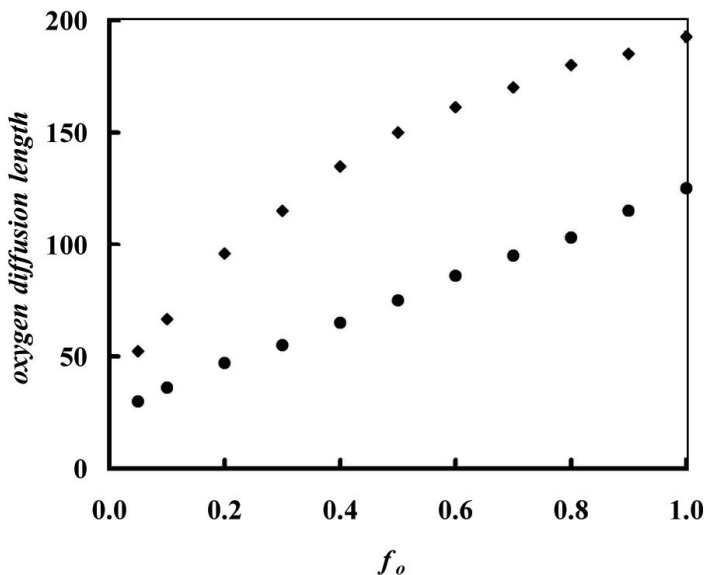


Figure 6: The diffusion length of the oxygen field versus the frequency of attempts f_O . The two curves were obtained with $S_H = 0.5$ (diamonds) and $S_H = 0.3$ (circles).

The above considerations suggest that the propagation of a burning front could be described, in a S_H, f_O plane, through a morphological phase diagram, where thinner structures (corresponding to dendritic-like patterns of the combustion front) should correspond to a large growth rate or low oxygen diffusivity, 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 $A_0 = 0.75$.

4 Conclusions

In the present paper we presented some numerical results obtained with a lattice model which describes the propagation of combustion in the absence of convection. We observed that the diffusive transport of oxygen is at the origin of a morphological instability of the combustion front. The process lacks a stabilization mechanism at the microscopic level, however the necessity to preserve adequate temperature conditions for the burning reaction results in a tendency to minimize the area of the advancing front, mimicking the effects of surface tension. The resulting pattern is characterized by a typical length scale which is related to the diffusion length of the oxygen and the heat fields. Even in partial defect of oxygen, the burning front can advance at constant growth rate as unburned fuel is left behind the advancing front. The numerical simulations carried out at various

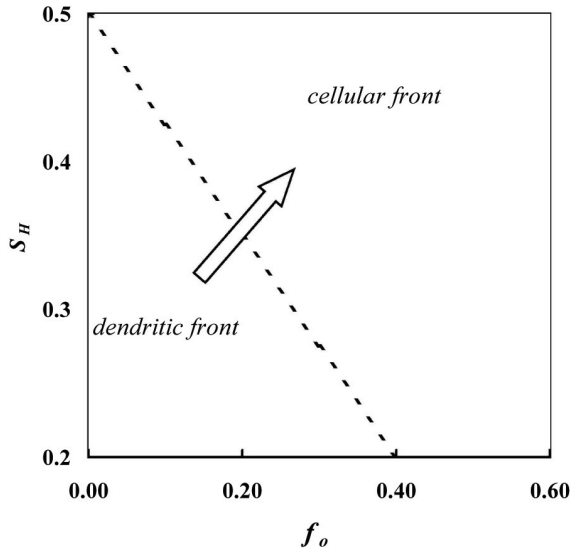


Figure 7: The morphological phase diagram for the pattern of the combustion field in the S_H, f_O plane.

diffusion rates display the complex morphology of the interfacial patterns and allowed us to construct a phase diagram of the phenomenon.

References

- [1] I. Glassman and R.A. Yetter, *Combustion* (Academic Press, Burlington MA, 2008).
- [2] J.S. Langer, *Instabilities and pattern formation in crystal growth*, Rev. Mod. Phys. 52,(1980), pp. 1–28.
- [3] W.W. Mullins, R.F. Sekerka *Morphological stability of a particle growing by diffusion and heat flow*, J. Appl. Phys, 34 (1963),pp. 323–329.
- [4] M. Conti, U. Marini Bettolo Marconi *Fingering in slow combustion*, Physica A, 312 (2002), pp. 381–391.
- [5] O. Zik, Z. Olami, E. Moses, *Fingering instability in combustion*, Phys. Rev. Lett. 81 (1998), pp. 3868–3871.
- [6] O. Zik, E. Moses, *Fingering instability in combustion:an extended view*, Phys. Rev. E 60 (1999), pp. 518–531.
- [7] M. Conti, U. Marini Bettolo Marconi *Novel Monte-Carlo lattice approach to rapid directional solidification of binary alloys*, Physica A, 277 (2000), pp. 35–46.