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Reaction–diffusion pulses: a combustion model

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Abstract

We focus on a reaction–diffusion approach proposed recently for experiments on combustion processes, where the heat released by combustion follows first-order reaction kinetics. This case allows us to perform an exhaustive analytical study. Specifically, we obtain the exact expressions for the speed of the thermal pulses, their maximum temperature and the condition of self-sustenance. Finally, we propose two generalizations of the model, namely, the case of several reactants burning together, and that of time-delayed heat conduction. We find an excellent agreement between our analytical results and simulations.

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1. Introduction

Reaction–diffusion (RD) equations may be written in the general form

$$\frac{\partial n(x,t)}{\partial t} = D(x,t)\frac{\partial^2 n(x,t)}{\partial x^2} + F(n,x,t) \tag{1}$$

where $n(x,t)$ is a density distribution function, D is the diffusion coefficient and $F(n,x,t)$ is a function accounting for production or annihilation processes. These sort of equations have attracted great attention from many different fields. Their main advantage lies in the fact that they admit travelling solutions $n(x,t) = n(x - vt)$, with v being the characteristic speed [1].

If we assume that the medium we are considering is homogeneous, as most works do [1–7], we can take the diffusion coefficient as a constant parameter. Then, the solution of equation (1) and the exact expression of v are determined solely by the form of F. Some well-known cases have been reported before.

(a) $F = an(1-n)$, with $a > 0$. In this case, equation (1) turns into the F-KPP equation, whose solutions have been widely studied [2, 3]. Wavefront solutions arise both from numerical simulations and theoretical analysis, and the wavefront speed v is found to follow the expression [2]

$$v = 2\sqrt{aD}. \tag{2}$$

There are many works that have proved the usefulness of this term on fields as population dynamics and ecology, as the logistic growth $n_t = an(1-n)$ shows a great ubiquity in natural systems. Some examples are biological invasions [4], human migrations [5], spread of viruses [6], etc.

(b) $F = -b(n-n_0) + A\,\mathrm{e}^{-E/Rn}$, with $b, k, E, R > 0$. This term has been used in some combustion models [8–11], n being the temperature of the system. The linear term concerns the heat lost by convection, while the second one comes from the Arrhenius law [8, 12]. As the exponential dependence on the rate constant is supported by experiments for many chemical processes (as combustion), its theoretical significance has also received great attention [12]. E and A have been traditionally called the activation energy and the pre-exponential factor, respectively. Nevertheless, the exact solution for this case (b) is not known and previous papers on this field have just given some approximations based on linearization methods [9, 10].

In this paper we are going to study analytically for the first time the case

$$F \sim -b(n-n_0) + c\,\mathrm{e}^{-\alpha t}H(t) \tag{3}$$

where $c, \alpha > 0$ and $H(t)$ is the Heaviside function. This expression has been proposed before for the modellization of combustion in two-dimensional fuel beds obtaining good agreement between simulations and experiments [13], therefore offering an interesting alternative to the well-known case (b). Nevertheless, there is a lack of analytical study for this model which we want to amend with this work.

The main advantage, in comparison to previous RD approaches, is that in this new case the temperature spreads as a travelling pulse. It is different to what happens in cases such as (b); there, the temperature reaches an asymptotic value for which the effects of convection and combustion are in equilibrium, and so the final solution is a travelling front (which implies that the reactants go on burning indefinitely). Thus, the approach we present here seems to give a more realistic approach for a combustion process. Moreover, this model presents potential applications to other systems in which pulses (rather than fronts) appear as a consequence of the consumption of one of the reactants (species), as chemical systems [14], predator–prey waves [1] or intracellular signal propagation [15].

This paper is organized as follows. In section 2 we present the general equations of our model and show how analytical solutions can be achieved by means of a piecewise description of the model. It leads us to exact expressions for the speed of thermal pulses, their maximum temperature and a critical condition for their self-sustenance (i.e. existence). Section 3 focuses on the more general case of several reactants burning together; in this case, we show that analytical solutions are still reached in the appropriate regime. In section 4 the classical conduction equation (based on Fick's law) is replaced by the Maxwell–Cattaneo expression, which involves delay effects; we also obtain the exact solution for this case similarly to that in section 2. Finally, section 5 is devoted to final conclusions.

2. The model

For convenience, we will analyse this model and the generalizations we propose below in terms of combustion processes. So, we use the temperature T as the main variable instead of n.

The derivation of the combustion term in our model comes from the assumption that the fuel burns at a constant rate α which is proportional to the fraction of the fuel remaining unreacted (first-order reaction). We then have that the fuel density ρ decreases at a given point according to

$$\rho = \rho_0 \, \mathrm{e}^{-\alpha t}. \tag{4}$$

Therefore, we can write

$$\frac{\partial T}{\partial t} = -Q\frac{\partial \rho}{\partial t} = Q\alpha\rho_0 \, \mathrm{e}^{-\alpha t} \tag{5}$$

where we define $Q \equiv Q^*/m$ as the quotient between the enthalpy of combustion Q^* per unit mass and the heat capacity m per unit area (considering a 2D system).

Finally, we introduce a Heaviside function for taking into account the fact that the combustion process at any given point starts just when the temperature there reaches a threshold value T_h, which is the ignition temperature. Then, our main equation can be written as

$$\frac{\partial T(x,t)}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2} - k(T - T_0) + Q\alpha\rho_0 \, \mathrm{e}^{-\alpha(t-t_h)} H(t - t_h). \tag{6}$$

The three terms on the right-hand side account for heat diffusion, heat interchanges by convection with the air (T_0 is the ambient temperature) and heat released by combustion, respectively. t_h can be interpreted as the time where the ignition temperature is reached at a given point of the media; so, t_h depends explicitly on the spatial variable x. We use the form $H(t - t_h)$ instead of $H(T - T_h)$ because it is more convenient from mathematical point of view, as we shall show below. We stress that such an approach has been proposed before for the modellization of combustion in two-dimensional fuel beds, obtaining good agreement between simulations and experiments [13], but no analytical expressions (i.e. for the pulse speed) have been previously derived.

We will use a method based on that presented recently by Theodorakis and Svoukis [16]. They took the dimensionless partial differential equation (PDE)

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + F(T) \tag{7}$$

and showed that when the production term $F(T)$ does not allow us to find analytic solutions, a good way for obtaining an approximate solution consists in a piecewise linear emulation of $F(T)$ and requiring the solution to be continuous and smooth everywhere. They also used the condition that the PDE must exhibit travelling solutions with constant speed v, as usual in RD equations.

We claim that the same ideas can be applied when the production function has a piece-like form as that in our model, where

$$\begin{aligned} &\text{(i)}\ F = -k(T - T_0) && \text{for} \quad t < t_h \\ &\text{(ii)}\ F = -k(T - T_0) + Q\alpha\rho_0 \, \mathrm{e}^{-\alpha(t-t_h)} && \text{for} \quad t > t_h. \end{aligned} \tag{8}$$

According to our arguments, we can solve (i) and (ii) separately and make both solutions continuous and smooth at $t = t_h$. By doing this, we expect to find an expression which gives us the explicit form of the speed v, as in [16].

2.1. General solution

First, we assume that travelling solutions (i.e. which propagate without changing shape and with constant speed v) arise from our model, so the variable $z = x - vt$ can be used instead of x and t. In consequence, it must be noted that our method (as most RD models) is restricted to those n-dimensional cases where the front has radial symmetry, so z can be defined properly, x being the distance to the origin. Now, if we define the variable $T^* \equiv T - T_0$ for simplicity, equation (6) becomes

$$\frac{\partial T^*}{\partial z} = D\frac{\partial^2 T^*}{\partial z^2} - kT^* + Q\alpha\rho_0 \,\mathrm{e}^{\frac{\alpha z}{v}} H(-z) \tag{9}$$

where we have considered that the position of the pulse at time t is determined by those points where the combustion starts at that moment, so $t - t_h = t - \frac{x}{v} = -\frac{z}{v}$. We separate the solution of the model into two parts (from now on, we will omit the asterisk in T^* for simplicity):

(i) $z > 0$. This region represents the points where combustion is yet to begin at a given time, so we have $F = -kT$ and the exact solution of the ordinary differential equation (ODE) can be found as

$$T(z) = A_1 \,\mathrm{e}^{m_+ z} + A_2 \,\mathrm{e}^{m_- z} \tag{10}$$

where

$$m_\pm = \frac{-v \pm \sqrt{v^2 + 4Dk}}{2D}. \tag{11}$$

It is worthwhile to note that in any case $m_+ > 0$ and $m_- < 0$. The values of the integration constants A_1 and A_2 will arise from the boundary conditions, which in this case are

$$T(\infty) = 0 \qquad T(0) = T_h. \tag{12}$$

Finally, we obtain

$$T(z) = T_h \,\mathrm{e}^{m_- z}. \tag{13}$$

(ii) $z < 0$. After combustion starts at a certain point, the last term in (9) is nonzero. Nevertheless, as the new term does not depend explicitly on T, the ODE can still be solved exactly, giving

$$T(z) = B_1 \,\mathrm{e}^{m_+ z} + B_2 \,\mathrm{e}^{m_- z} + \Omega \,\mathrm{e}^{\frac{\alpha z}{v}} \tag{14}$$

where

$$\Omega = \frac{Q\alpha\rho_0 v^2}{(k - \alpha)\, v^2 - D\alpha^2}. \tag{15}$$

For this second region, the boundary conditions are

$$T(-\infty) = 0 \qquad T(0) = T_h \tag{16}$$

so we have

$$T(z) = T_h \,\mathrm{e}^{m_+ z} + \Omega\left(\mathrm{e}^{\frac{\alpha z}{v}} - \mathrm{e}^{m_+ z}\right). \tag{17}$$

To obtain this solution we have implicitly used the condition that T is continuous at $z = 0$ by means of the ignition temperature T_h. According to our discussion above, we still require the smoothness of the solution at $z = 0$. From this extra condition, we will find an expression that will allow us to determine the velocity. Equalling the derivatives of $T(z)$ in the two regions at $z = 0$ leads us to the relation

$$T_h(m_- - m_+) = \Omega\left(\frac{\alpha}{v} - m_+\right). \tag{18}$$

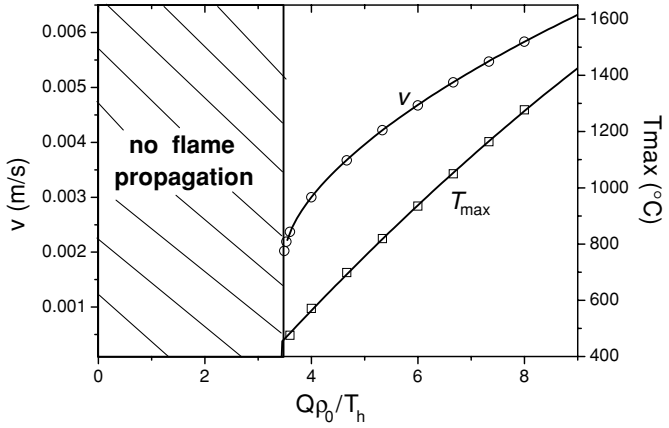

Figure 1. Comparison between simulations (symbols) and theory (line) for the pulse speed v (circles) and $T_{\max}$ (squares) as a function of the adimensional number $Q\rho_0/T_h$. The figure also shows the threshold below which pulses cannot propagate. In this and all of the other figures, the values of the parameters used in the simulations are those estimated in [13], i.e. $Q = 3605\ \mathrm{m^2\ C\ kg^{-1}}, k = 0.071\ \mathrm{s^{-1}}, D = 3.1 \times 10^{-5}\ \mathrm{m^2\ s^{-1}}, \alpha = 0.19\ \mathrm{s^{-1}}, \rho = 0.4\ \mathrm{kg\ m^{-2}}$, $T_h = 300\ ^\circ\mathrm{C}$.

Equation (18) gives an expression for v as a function of the parameters of the model. Nevertheless, as $m_\pm$ and Ω depend on v in a complicated way, the explicit expression for the velocity cannot be given easily. So, we will take (18) as the general expression for v. However, analytical calculus from (18) allows us to find the condition required for obtaining real positive values of v; it will be the condition for the existence of travelling pulses. We find that this condition has the form

$$\frac{Q\rho_0}{T_h} > 1 + \frac{2(k + \sqrt{2k\alpha})}{\alpha} \equiv \left(\frac{Q\rho_0}{T_h}\right)_{\mathrm{cr}}. \tag{19}$$

This condition is noteworthy from the experimental point of view as from the characteristics of the system and the fuel chosen we can know the minimum initial density ρ_0 needed for obtaining a self-sustained propagative process. Under the critical threshold, the amount of heat released by chemical reactions is not sufficient to heat new reactants up to the ignition temperature, so propagation is not possible.

Finally, we will predict analytically the maximum temperature ($T_{\max}$) of the pulse, as there are many real cases in which this parameter is of great interest, specially for safety purposes. As the peak of the pulse is reached for $z < 0$ we must now use just the solution from the region (ii). We can obtain easily through the derivative of equation (17) that the general expression for $T_{\max}$ is

$$T_{\max} = (T_h - \Omega)\left(\frac{\Omega\alpha}{vm_+(T_h - \Omega)}\right)^{\frac{m_+}{m_+ - \alpha/v}} + \Omega\left(\frac{\Omega\alpha}{vm_+(T_h - \Omega)}\right)^{\frac{\alpha/v}{m_+ - \alpha/v}}. \tag{20}$$

The validity of these expressions was analysed by comparing them with simulations of equation (6). In the simulations, we started from the initial conditions

$$\begin{aligned} T &= T_h \qquad \text{for} \quad x < x_0 \\ T &= 0 \qquad \text{for} \quad x > x_0 \end{aligned} \tag{21}$$

i.e. we supposed that the combustion process started at $t = 0$ in a little domain of the media (which has to be great enough to allow the formation of the pulses), while the rest was still at the ambient temperature. In figure 1 we have performed a comparison between

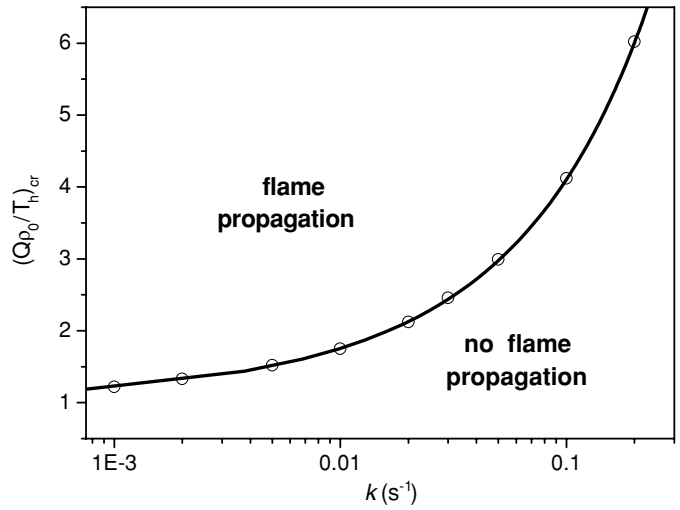

Figure 2. Plot of the *no-propagation* threshold $(Q\rho_0/T_h)_{\rm cr}$ as a function of the convection parameter k. The solid line corresponds to equation (19), while the circles arise from simulations.

equations (18)–(20) and the values obtained for the velocity of pulses and the maximum temperature from simulations, achieving an excellent agreement. The values of the parameters used in this plot and the others below are those estimated from the experiments in [13].

The *propagation condition* has also been tested by letting the pulses evolve for large times. For values below the threshold value, pulses finally vanished (the time pulses needed to vanish depends on the value of x_0 chosen), while for values above the threshold the pulses asymptotically reached a constant shape (according to the requirement of travelling solutions). Figure 2 shows the agreement found between these simulated processes and equation (19).

2.2. Case $k = 0$

When the convection term is neglected, the production function reduces just to the combustion term. This case is very similar to F having the Lipschitz form [17], where F is zero for temperatures lower than a threshold T_h and positive above the threshold.

The main difference with the general case analysed above is that now heat is not dissipated by the system, so now the temperature does not decrease for large times and travelling fronts arise instead of pulses, as can be seen in figure 3. So, this specific case allows us to illustrate one of the main features of the model, i.e, that the heat released by combustion decreases continuously, and so due to convection (when $k > 0$) the flames die out asymptotically.

For $k = 0$, our expression (18) turns into the simplified form

$$-\frac{T_h v}{D} = \frac{\Omega\alpha}{v} \tag{22}$$

which now allows us to isolate v, obtaining then

$$v = \sqrt{\frac{D\alpha(Q\rho_0 - T_h)}{T_h}}. \tag{23}$$

We show the results for $k = 0$ because this specific case has been studied before in many models [8, 10] (although it is not realistic in most cases) and because an elegant analytic

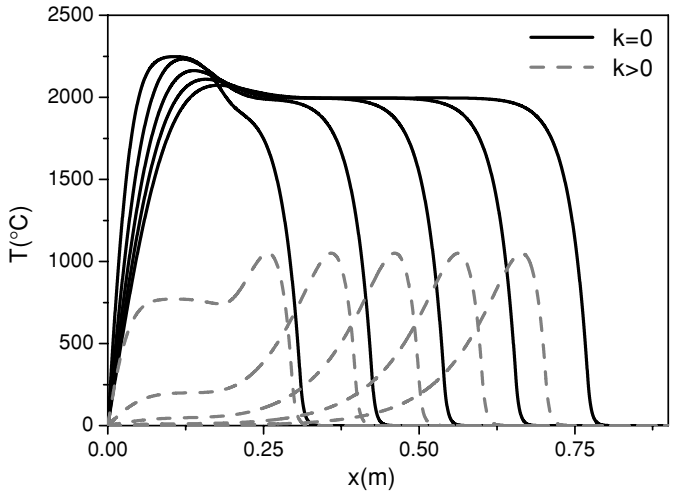

Figure 3. Evolution in time of the temperature profile from simulations, with the solutions travelling in the direction of the positive x axis. For the case with heat loss, $k > 0$ (dashed lines), a travelling pulse arises, while in the case without heat loss, $k = 0$ (solid lines), the solution has the form of a front.

expression for the velocity is found. Likewise, the condition for the existence of pulses and the expression for $T_{\max}$ become

$$\frac{Q\rho_0}{T_h} > 1 \tag{24}$$

$$T_{\max} = T_h - \Omega. \tag{25}$$

3. Model for several species

We can extend our arguments for the case in which two or more species can burn, each characterized by its own parameters Q_i, ρ_{0i}, α_i and T_{hi}. This is an interesting case for those experimentalists working on combustion of fuel beds with different mixed materials, or also for the modellization of a single material made up of different reactants, as is usual in real systems (wood, for example, usually contains 50–65% of cellulose, 20–35% of lignin and 5–15% of other components [18]).

Let us study the case of two species. The main difficulty when different fuels are considered is that ignition temperatures (T_{h1} and T_{h2}) are also different, so combustion of each one does not start at the same moment. Then, a new parameter τ must be considered, which is the time since one of the fuels starts burning till the second one does. The general equation will then read

$$\frac{\partial T}{\partial z} = D\frac{\partial^2 T}{\partial z^2} - kT + Q_1\alpha_1\rho_{01}\,\mathrm{e}^{-\frac{\alpha z}{v}}H(z) + Q_2\alpha_2\rho_{02}\,\mathrm{e}^{\alpha\left(\frac{z}{v}-\tau\right)}H\left(\frac{-z}{v}-\tau\right). \tag{26}$$

We can now use the same method for finding v that was used in the first section, but now three different regions must be considered, i.e. (i) before combustion starts, (ii) when only one of the species has reacted and (iii) when both species are burning. The boundary conditions we impose are

$$T(\infty) = 0 \qquad T(-\infty) = 0 \qquad T(0) = T_{h1} \qquad T(-\tau v) = T_{h2}. \tag{27}$$

(i) $z > 0$. Analogously to the region (i) in the section 2, we obtain

$$T(z) = T_{h1}\,\mathrm{e}^{m_- z}. \tag{28}$$

(ii) $-\tau v < z < 0$. Now the first combustion term in (26) must be considered, so the exact solution of the ODE is

$$T(z) = B_1\,\mathrm{e}^{m_+ z} + B_2\,\mathrm{e}^{m_- z} + \Omega_1\,\mathrm{e}^{\frac{\alpha_1 z}{v}}. \tag{29}$$

(iii) $z < -\tau v$. When both combustion terms are included the solution is

$$T(z) = (T_{h2} - \Omega_1\,\mathrm{e}^{-\alpha_1\tau} - \Omega_2\,\mathrm{e}^{-\alpha_2\tau})\,\mathrm{e}^{m_+(z+\tau v)} + \Omega_1\,\mathrm{e}^{\frac{\alpha_1 z}{v}} + \Omega_2\,\mathrm{e}^{\frac{\alpha_2 z}{v}} \tag{30}$$

where we define

$$\Omega_i = \frac{Q_i \alpha_i \rho_{0i} v^2}{(k - \alpha_i)v^2 - D\alpha_i^2} \tag{31}$$

$$B_1 = \frac{T_{h2} - \Omega_1\,\mathrm{e}^{-\alpha_1\tau} + (\Omega_1 - T_{h1})\,\mathrm{e}^{-\tau v m_-}}{\mathrm{e}^{-\tau v m_+} - \mathrm{e}^{-\tau v m_-}} \tag{32}$$

$$B_2 = \frac{T_{h2} - \Omega_1\,\mathrm{e}^{-\alpha_1\tau} + (\Omega_1 - T_{h1})\,\mathrm{e}^{-\tau v m_+}}{\mathrm{e}^{-\tau v m_-} - \mathrm{e}^{-\tau v m_+}}. \tag{33}$$

As our solution is divided into three regions, we now have to require the smoothness of it at two different points ($z = 0$ and $z = -\tau v$). From the two resultant expressions we will obtain a system to determine the front speed v and the transition time τ. However, if one tries to solve that system in the general case, the expressions that arise are enormous. A simplification can be done by recovering the condition that the solutions we are considering have the form of a steep pulse. Then, the time τ is expected to be very small ($\tau \ll 1$), so we can neglect from our derivation the terms of order $O(\tau^2)$. By doing so, the following expressions arise:

$$\tau = \frac{T_{h1} - T_{h2}}{v T_{h1} m_-} \tag{34}$$

$$v m_+(\Omega_1 + \Omega_2) = \Omega_1\alpha_1 + \Omega_2\alpha_2 + v(m_+ T_{h1} - m_- T_{h2}). \tag{35}$$

As happened with (18), again equation (35) leads us to a really complicated explicit expression for v. Thus, we prefer to take (35) as our general solution.

It is also important in this case to analyse the result for the time τ. We have supposed that the transition time should be small, but one can see from equation (34) that in general this condition will only be true when $(T_{h2} - T_{h1}) \ll T_{h1}$. Thus, our solution will only hold for those cases where the relative difference between the ignition temperatures is small. Figure 4 shows the results for equation (35) and its link to this limiting restriction on the ignition temperatures. We obtain, as expected, that in the regime $(T_{h2} - T_{h1}) \ll T_{h1}$ the result found agrees well with the pulse speed from simulations, but when this condition no longer holds, clear differences appear.

However, we note that, despite this limitation, the model is still useful for many real systems, as ignition temperatures for many kinds of organic fuels and woods are similar [18]. In the opposite case, when $\tau \ll 1$ does not hold, we then have that T_{h2} is much higher than T_{h1} and the speed of the front will decrease progressively. Finally, there would be a critical T_{h2} for which the amount of heat released by the first reactant would not be sufficient to reach T_{h2} and so only the first reactant would burn; then, we would have a case equivalent to that in section 2 with the front speed determined by (18). This behaviour for large T_{h2} is confirmed by our simulations and also shown in figure 4 (where, the dotted line represents the value for the speed assuming that only the first reactant is present).

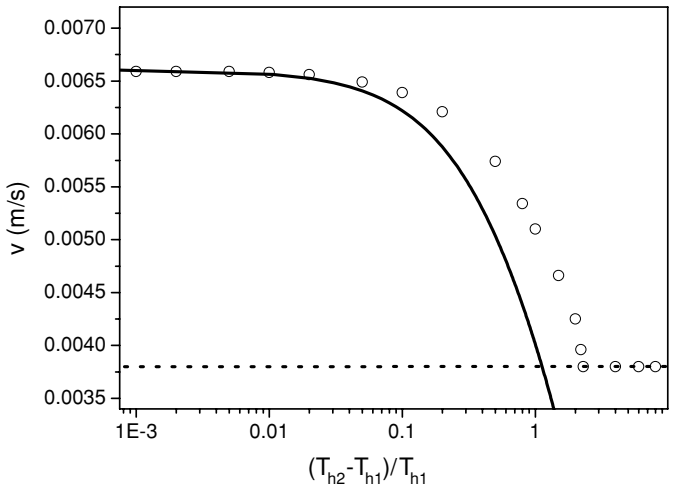

Figure 4. Two-species model. Comparison between simulations (circles) and theory (solid line) for the pulse speed as a function of $(T_{h2} - T_{h1})/T_{h1}$. As argued in the text, the analytic solution found is only valid when the condition $(T_{h2} - T_{h1}) \ll T_{h1}$ holds. For large $(T_{h2} - T_{h1})/T_{h1}$, the speed has the same value as if only the first reactant were present (dotted line).

4. Maxwell–Cattaneo model

We still propose another generalization of the model by considering the possibility that the heat diffusion is governed by the Maxwell–Cattaneo equation

$$u\frac{\partial q}{\partial t} + q = -D\frac{\partial T}{\partial x} \tag{36}$$

instead of the usual Fourier law ($u = 0$), according to the extended irreversible thermodynamics [19]. In this equation, q is the flux of heat in the x direction and u represents a time delay which implies relaxational effects on the heat diffusion process, and so it offers a possible solution to the problem of infinite speed of thermal signals detected for the Fourier law [20]. There have been different discussions about the correct way of introducing the delay u in physical systems [21, 22] and so the validity of the Maxwell–Cattaneo expression is still an open field; specifically, some criticisms against it argue that it is not frame-invariant and so is not a suitable physical law. An interesting generalization of (36) is proposed in [21] and more comments about the problem of frame invariance can be found in [19] (p 32). However, we stress that some previous works on combustion have already explored the Maxwell–Cattaneo approximation, achieving interesting results [7, 9], so we consider it worthwhile to analyse it.

When we combine equation (36) and the energy balance equation

$$\frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = F \tag{37}$$

the hyperbolic RD equation arises [23],

$$\frac{\partial T}{\partial t} + u\frac{\partial^2 T}{\partial t^2} = D\frac{\partial^2 T}{\partial x^2} + F + u\frac{\partial F}{\partial t}. \tag{38}$$

For the specific case we are considering and writing the equation in terms of the variable z, we obtain

$$(D - uv^2)\frac{\partial^2 T}{\partial z^2} + v(1 + uk)\frac{\partial T}{\partial z} - kT + \alpha Q\rho_0(1 - u\alpha)\,\mathrm{e}^{\frac{\alpha z}{v}}H(-z) = 0. \tag{39}$$

We can now easily solve this equation if we redefine our parameters in the following way:

$$D^{\dagger} = \frac{D - uv^2}{1 + uk} \tag{40}$$

$$k^{\dagger} = \frac{k}{1 + uk} \tag{41}$$

$$Q^{\dagger} = Q\frac{1 - u\alpha}{1 + uk}. \tag{42}$$

Then, it may be seen that equation (39) is exactly the same as (9). Hence, we do not need to present again the whole solution, as the boundary conditions are the same too (the delay does not change the properties of combustion, which just depend on the absolute value of T; so, we still have $T = T_h$ at $z = 0$). For the general case, we will obtain that the implicit expression of v is, analogous to (18),

$$T_h\left(m_-^{\dagger} - m_+^{\dagger}\right) = \Omega^{\dagger}\left(\frac{\alpha}{v} - m_+^{\dagger}\right) \tag{43}$$

where the new quantities with index † are defined as those in section 2, with $D^{\dagger}$, $k^{\dagger}$, $Q^{\dagger}$ instead of D, k, Q.

It must be pointed out that the equivalence between (39) and (9) presents some limitations. Actually, we need to impose that the parameters in our model are positive in order to ensure the robustness of the method; so, from (40)–(42) we get some restrictions for the value of u,

$$u < \frac{1}{\alpha} \qquad u < \frac{D}{v^2}. \tag{44}$$

The case $k = 0$ allows us to find an explicit expression again, which now reads

$$v = \sqrt{\frac{D\alpha(Q\rho_0(1 - u\alpha) - T_h)}{(1 - u\alpha)(T_h + \alpha Q\rho_0 u)}}. \tag{45}$$

Likewise, the delay u also alters the threshold parameters for which the pulses are self-sustained. By analytical calculus, from equation (43) one finds that the real solutions for v are only possible in the regime

$$\frac{Q\rho_0}{T_h} > \frac{\alpha(1 + uk) + 2\left(k + \sqrt{2k\alpha(1 + uk)}\right)}{\alpha(1 - u\alpha)} \equiv \left(\frac{Q\rho_0}{T_h}\right)_{\mathrm{cr}} \tag{46}$$

and if we consider the limiting case of no convection losses ($k = 0$),

$$\frac{Q\rho_0}{T_h} > \frac{1}{1 - u\alpha}. \tag{47}$$

Figures 5 and 6 are equivalent to figures 1 and 2. According to them, the agreement found between our analytical expressions ((43) and (46)) and simulations from the general PDE is excellent. Moreover, these plots allow us to observe very clearly the effect of introducing the time delay u on the system. We see that two consequences arise: (i) the speed of the pulses decreases as the delay u increases, in accordance with other RD models based on the Maxwell–Cattaneo expression [7, 23] and (ii) the threshold $(Q\rho_0/T_h)_{\mathrm{cr}}$ increases with u, so the *propagation condition* becomes more restrictive. Both consequences agree with the intuitive idea that under relaxational effects the diffusion process cannot be as efficient as in the non-delayed case, since equation (36) implies that a finite time is required by the system to respond to the thermal gradient.

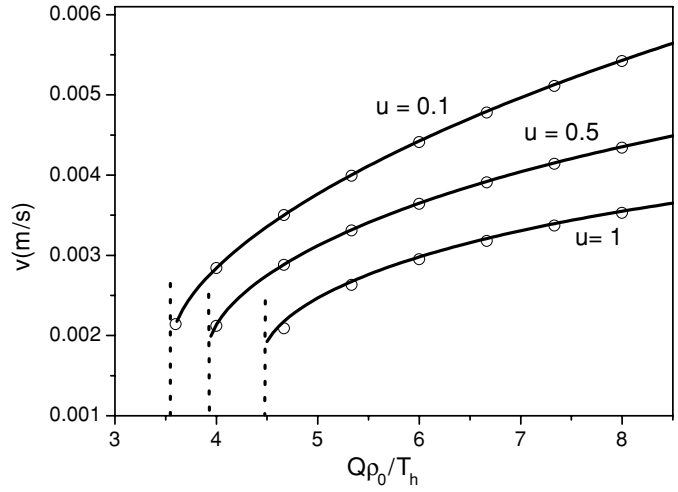

Figure 5. Comparison between simulations (points) and theory (line) for the pulse speed as a function of the adimensional number $Q\rho_0/T_h$ for different time delays u in the Maxwell–Cattaneo model. The vertical lines determine the *no-propagation* threshold for every case.

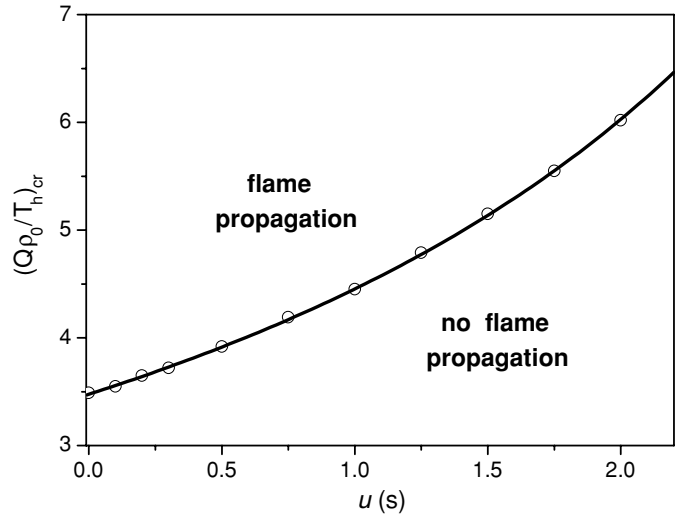

Figure 6. Plot of the no-propagation threshold $(Q\rho_0/T_h)_{\rm cr}$ as a function of the time delay u for the Maxwell–Cattaneo model. The solid line corresponds to equation (19) and the points arise from simulations.

5. Summary

We have studied analytically for the first time a RD model where the reaction term follows first-order kinetics with a constant rate α plus convection losses. This model has been shown before to be of particular interest for the modellization of temperature pulses travelling on fuel beds [13]. From the agreement found in those works with experiments, one may conclude that this new model (1)–(3) can be a good alternative to the usual Arrhenius law that many theoretical works have considered before [8–10]. Specifically, the fact that these kind of RD

models are continuous and the assumption we have made that the initial density of reactants ρ_0 is a constant, make us think that the model can be of special interest for systems where the reactants are distributed homogeneously, as fuel beds or dense forests.

The main goal of our study has been to determine the speed and maximum temperature of travelling pulses arising from the model and the conditions for the self-sustenance of these pulses. Mathematically, we have used the ideas by Theodorakis and Svoukis for finding travelling solutions of a PDE. They found that for a linear piece-like production function $F(T)$, the speed selected by the travelling front arises from the condition that the solutions must be continuous and smooth everywhere. Here, we have extended these arguments to the case when F is a piece-linear function in time (instead of the main variable T) and for the case of travelling pulses instead of fronts; so, the condition $T(-\infty) = T_{\max}$ they used has been replaced here by $T(\infty) = 0$ (as the fuel becomes exhausted, the heat released by combustion decreases with time and the system returns to the initial state far behind the pulse).

In addition, we have considered some possible generalizations of the model which can be of interest to scientists working on different topics. When several reactants are considered, we have seen that there is still an analytical solution from which the speed of the pulse can be found. This case can be of great interest when different mixed materials burning together have to be modellized, as mentioned above, but it also allows the possible application to forest fires with different kinds of trees burning (or taking into account combustion of high trees plus bushfire combustion near the land).

The model in the third section, based on the ideas of the extended irreversible thermodynamics, involves delay effects on the diffusion process. As one intuitively expects, when the delay is considered, the pulses are slower and the condition of self-sustenance is more restrictive. Hence, we think that this model can offer a new possibility to experimentalists for determining if the Maxwell–Cattaneo equation is appropriate for physical systems and so it could help to solve the present controversy.

Finally, there are still many possibilities of improving this model that we have not explored yet. New terms can be added by taking into account heat radiation, interaction between the different reactants, the effects of heterogeneities, etc. We shall develop these ideas in further works.

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