Etude d'une équation de convection-réaction-diffusion en écoulement compressible

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Résumé. Nous avons étudié la propagation d'un front de flamme dans une configuration unidimensionnelle en solvant numériquement une équation de advection-diffusion-réaction (ADR). Nous avons choisi un modèle simplifié dans lequel le couplage avec d'autres phenomènes est négligé et le fluide réactant est une mixture de gaz. En outre, la vitesse de l'écoulement compressible est donné de façon analytique. A l'aide de la simulation numérique nous analysons la différence entre différents modéles qui sont communement utilisés dans les études fondamentales en combustion et en biologie. Puis nous avons caracterisé l'effet de la compressibilité sur la dynamique du front et dans quelles conditions il est possible que la flamme s'eteigne avant la saturation de la réaction.

Abstract. We have studied the front propagation in a one dimensional case of combustion by solving numerically an advection-reaction-diffusion equation. The physical model is siplified so that no coupling phenomena are considered and the reacting fluid is a binary mixture of gas. The compressible flow field is given analitycally. We analyse the differences between popular models used in fundamental studies of compressible combustion and biological problems. Then, we investigate the effects of compressibility on the front interface dynamics for different reaction types and we characterise the conditioins for which the reaction stops before its completion.

1 Introduction

Transport of reacting species advected by laminar or turbulent flows described by an advection reaction diffusion equation (ARD), is an issue of interest in many fields, e.g., population dynamics, propagation of plankton in oceanic currents, reacting chemicals in the atmosphere, ozone dynamics, complex chemical reactions, and combustion. While these phenomena have been and are being widely studied in the case of incompressible flows, the transport of reactive species advected by compressible flows is less discussed. Only recently has been extended to the study of population dynamics [1]. Combustion processes are particularly complex because they involve a large number of chemical species and a large number of reactions. In addition, the concentration of these species, and the release of chemical energy during reactions, greatly affect the flow field of the fuel and oxidizer mixture. Consequently, the numerical study of this phenomenon requires the solution of a large number of coupled partial difference equations (conservation of species, momentum conservation and energy conservation).

The complexity can be greatly reduced if we minimize the physical details. In particular, if we neglect the effects of the coupling between the various equations and we minimize the number of species, combustion can be described approximately by an advection reaction diffusion equation :

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\gamma \nabla \phi) + s \qquad (1)$$

which describes the spatio-temporal behavior of a fraction ϕ of the reactive mixture which moves with velocity $\mathbf{u}$. The mean density of the mixture is ρ, $\gamma = \rho D$ is the diffusion coefficient and s is the source term.

Although there is a strong connection between the study of population dynamics and combustion, as the simplified mathematical model is equivalent when we consider incompressible flows, in the case of compressible flows we will show briefly that the parallelism requires a little more attention.

2   Model

If we consider a compressible reactive flow, and if the fluid is a mixture of N perfect gas, the local total mass balance over a volume V gives

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{2}$$

where $\rho(\mathbf{x}, t) = \sum_k \rho_k$ is the density of the mixture and $\mathbf{u}(\mathbf{x}, t)$ is the resultant velocity field [2,3]. This equation is the summation over the N mass species conservation

$$\frac{\partial \rho c_k}{\partial t} + \nabla \cdot [\rho(\mathbf{u} + \mathbf{v}_k) c_k] = R_k \qquad (k = 1, ..., N) \tag{3}$$

where $c_k(\mathbf{x}, t)$ is the mass fraction (ρ_k/ρ), $\mathbf{v}_k(\mathbf{x}, t)$ and R_k are the diffusion velocity and the reaction rate of the kth species, respectively. Of course, by definition, $\sum_{k=1}^{N} R_k = \sum_{k=1}^{N} \mathbf{v}_k c_k = 0$ as mass cannot be generated during chemical reactions.

If the mixture contains only two species, the pressure gradients are small, and volume forces are neglected [2]. Equation (3) for the kth species can be expressed as

$$\rho \frac{dc_k}{dt} = \rho \left[\frac{\partial c_k}{\partial t} + \mathbf{u} \cdot \nabla c_k \right] = \nabla \cdot (\rho D \nabla c_k) + R_k \qquad (k = 1, 2) \tag{4}$$

where the diffusion velocity is rewritten according to Fick's law. Equation (4) describe the spatio-temporal behavior of the fractions (c_1, c_2) of a binary reacting mixture in a compressible velocity field. Such as, for example, the fresh air as well as the burnt gas in a combustion reaction. If D is constant, equation (4) in conservative form becomes

$$\frac{\partial \rho c_k}{\partial t} + \nabla \cdot (\rho \mathbf{u} c_k) = D \nabla \cdot (\rho \nabla c_k) + R_k \qquad (k = 1, 2) \,. \tag{5}$$

If D and ρ are constant, equation (4) becomes the widely studied incompressible advection-reaction-diffusion equation with constant diffusion coefficient. Equations (4) and (5) differ from the equation

$$\frac{\partial \theta}{\partial t} + \nabla \cdot (\mathbf{u}\theta) = D_0 \nabla^2 \theta + F(\theta) \tag{6}$$

which is often found in literature [1,4] to describe the advection, diffusion and reaction of a scalar in a compressible flow. This equation is typical for studying the population dynamics and the scalar $\theta(\mathbf{x}, t)$, which is the concentration of a population [1]. However, this model is not correct for the concentration of combustion products. In fact, in equation (6), if $\nabla \cdot \mathbf{u} \neq 0$, the concentration θ can take values greater than one because this is not a fractional parameter. Notably if one considers the Fisher-Kolmogorov-Petrovskii-Piskunov reaction rate (FKPP) [5], the rate of grow $(F(\theta) = \alpha c(1 - c))$ in equation (6), if not correctly rescaled, can take negative values. This could be in agreement with the population dynamics point of view but is formally incorrect for the chemical reactions during a combustion.

2.1   Problem statement and numerical details

We have considered for simplicity a one dimensional case in which there is no feedback from the reaction rate, to the velocity field of the mixture. The velocity field is steady state and analytical so that the total mass balance becomes

$$\frac{\partial \rho u}{\partial x} = 0 \quad \rightarrow \quad \rho u = \rho \left[1 + U_0 \sin(\frac{\pi x}{L}) \right] = constant = \beta = 1 \tag{7}$$

where U_0 is a parameter defined on the interval $[0, 1]$ and $L = 1$ is the length scale of the velocity field. As shown in Fig. 1, when $U_0 = 0$ the mixture moves with constant velocity, the density is constant and
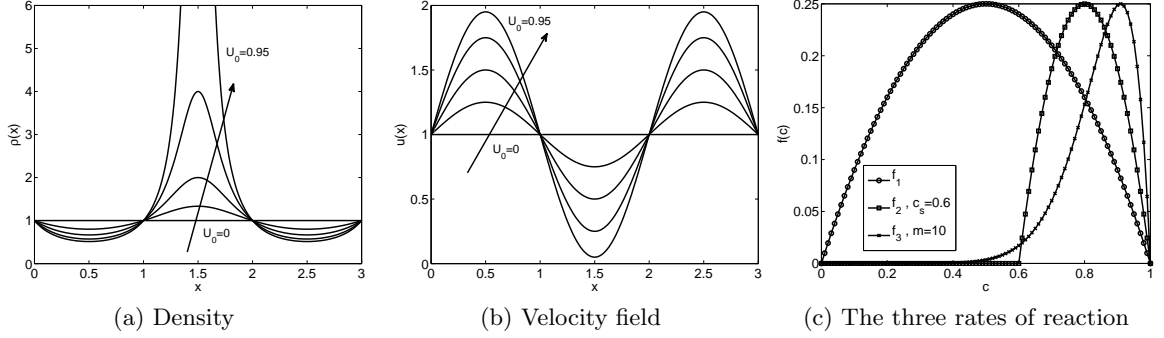
(a) Density   (b) Velocity field   (c) The three rates of reaction

FIG. 1. Density (a) and velocity field (b) of the mixture as function of parameter U_0. In (c) the three rates of reaction considered as function of the mass fraction : the FKPP reaction (f_1); the ignition type reaction (f_2) with threshold $c_s = 0.6$ and the general mth order Fisher reaction (f_3) with $m = 10$.

the problem becomes incompressible. On the other hand if U_0 tends to one the density varies very rapidly between 0.5 and the infinity.

If we consider the product $\rho D = \gamma$ constant and we collect and replace the velocity u with its analytic function, equation (4) becomes

$$\frac{\partial c}{\partial t} = \left[1 + U_0 \sin(\frac{\pi x}{L})\right] \left(\frac{\gamma}{\beta}\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x}\right) + f(c). \tag{8}$$

In this case, and later on, we will refer to $c(x,t)$ as the mass fraction of the reacted products, like the mass fraction of burnt gas in a combustion reaction. If only D is constant the balance equation for the burnt gas (5) gives :

$$\frac{\partial c^+}{\partial t} = u\left[\frac{D}{\beta}\frac{\partial}{\partial x}\left(\rho\frac{\partial c^+}{\partial x}\right) - \frac{\partial c^+}{\partial x}\right] + f(c^+). \tag{9}$$

If we use equation (6) instead, we will get the following one-dimensional ARD equation

$$\frac{\partial \theta}{\partial t} = D\frac{\partial^2 \theta}{\partial x^2} - u\frac{\partial \theta}{\partial x} - \theta\frac{\partial u}{\partial x} + f(\theta). \tag{10}$$

We will consider three different non-linear rates of reaction, as shown in Fig. 1c. The FKPP non linear rate of reaction or autocatalytic reaction is

$$f_1(c) = \alpha_1 c(1-c). \tag{11}$$

The ignition type rate of reaction is

$$f_2(c) = \begin{vmatrix} 0 & \text{if } c \leq c_s \\ \alpha_2(c-c_s)(1-c) & \text{if } c > c_s \end{vmatrix} \tag{12}$$

and the general mth order Fisher's non-linearity :

$$f_3(c) = \alpha_3 c^m (1-c). \tag{13}$$

If we use equations (8) and (9) c is defined in the interval $[0,1]$. The reaction rates then, by definition, are always positives or zero which means that the reaction is irreversible. As we will show soon this is not true for equation (6). The constants α_1, α_2 and α_3 are chosen so that $\max(f_i(c)) = \alpha_1/4$. In this way reactions have different reaction rates but with comparable characteristic times. Equations (8), (9) and (10) have been solved numerically using a fourth order finite different scheme for spatial discretization and a fourth order Runge-Kutta method for time advancement. The numerical domain has a dimension $L_x = nL$, where n is an even natural number, and periodic boundary condition have been applied.

3   Results

First of all we are interested in how the compressibility affects the time and the spatial behaviour of the fraction of burnt gas. We will solve now equation (8) setting up an initial condition for $c(x,t)$ as :

$$c(x, t = 0) = \exp\left[\frac{-(x - x_0)^2}{\sigma_0}\right] . \tag{14}$$

Results are shown in Fig. 2. If we focus just the front interface, it is possible to identify a general behavior : when $U_0 = 0$, the test case collapses to an incompressible advection-diffusion-reaction case where $u(x,t) = 1$ and $D_0 = \frac{\gamma}{\beta} = \gamma$ (as $\beta = 1$). Therefore, the burnt fraction moves with a constant velocity while it diffuses. The front interface is smooth end follows an exponential law.
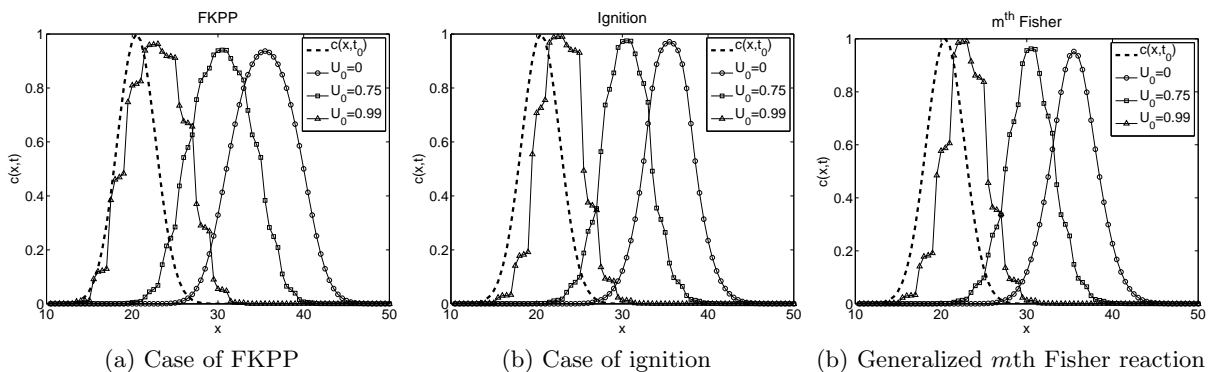

FKPP	Ignition	m^{th} Fisher
(a) Case of FKPP	(b) Case of ignition	(b) Generalized mth Fisher reaction

FIG. 2. In contiunous line, the mass fraction of burnt gas after a transient of $t = 15$. In dashed line the initial condition where $x_0 = 20.5$ and $\sigma_0 = 10$. Parameter $\frac{\gamma}{\beta} = 0.1$ ($\beta = 1, \gamma = 0.1$) and coefficient $\alpha_1 = 0.1$ are such that the maximum rate of reaction is $max(f_i) = 0.025$. In the case of ignition reaction the threshold was set up $c_s = 0.6$ while the exponent on the general Fisher non linearity is $m = 10$. Having fixed the grid step $dx = 0.025$ and the time step $dt = 0.0005$ we have run different simulations varying the coefficient U_0.

By increasing U_0 the front interface becomes more and more uneven. When U_0 tends to one, it becomes discontinuous. Moreover, the barycentric velocity of burnt fraction decreases by increasing U_0. These simulations were then repeated by solving equations (8) and (10) in the case of FKPP reaction (Fig. 3). We set up in both cases $D = \gamma = 0.1$ and the initial condition $c(x,t_0) = c^+(x,t_0) = \theta(x,t_0)$. The numerical method can be said to be validated since the three models are completely equivalent when $U_0 = 0$, where the three equations degenerate in the case of incompressible flow. Moreover, increasing U_0 but keeping it fairly low, there are no particular differences between the results obtained from equations (8) and (10). In this range of U_0, the hypothesis ρD constant is not far from the hypothesis D constant. Nevertheless results are different from those obtained through the model represented by equation (10). Peaks of the concentration appear in proximity of the density peaks of the fluid. Increasing U_0, we increase the compressibility and the concentration appears more and more peaked. Here, θ has values higher than the unity and hence confirming that in such areas the reaction rate is negative. For U_0 tending to unity, the differences between the three equations are particularly marked. The diffusion model becomes particularly important since it is found, as expected, a relevant difference between the results from equations (8) and (9).

We consider now the ignition reaction and we study under which conditon the reaction blows off. That is when the reaction stops before beeing completed. The phenomena can be studied by following in time the mass fraction of burnt gas which is defined, in normalized form, as :

$$m_b(t) = \frac{\int_0^{L_x} c(x,t)\rho(x)dx}{\int_0^{L_x} \rho(x)dx} . \tag{15}$$

(a) Equation (10) : $D = \gamma = 0.1$ (b) Equation (9) : $D = \gamma = 0.1$ (c) Equation (8) : $\rho D = \gamma = 0.1$
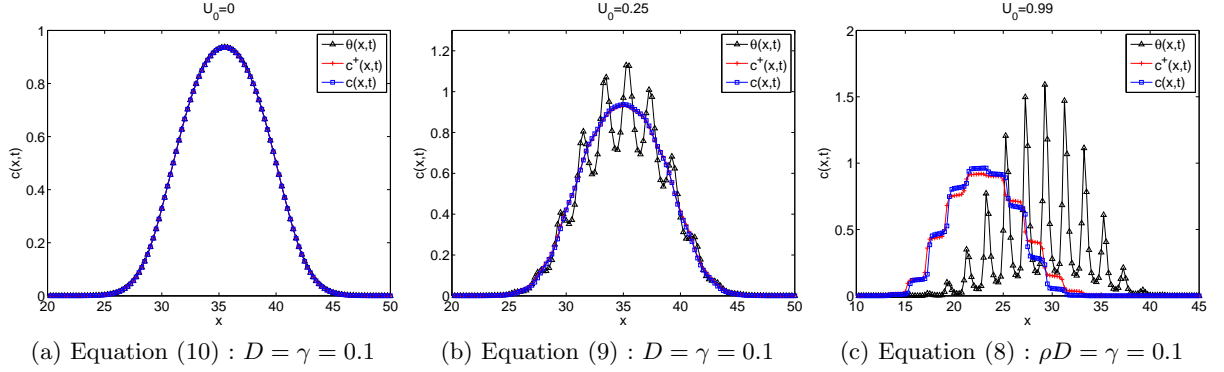
FIG. **3.** Comparison between results from equations (10), (9) and (8) after a transient of $t = 15$ by increasing U_0. The reaction rate is an FKPP type, the initial condition $c(x, t_0) = c^+(x, t_0) = \theta(x, t_0)$ with $x_0 = 20.5$ and $\sigma_0 = 10$, the grid step $dx = 0.025$ and the time step $dt = 0.0005$.

If the reaction does not blow off, m_b saturates to one. Otherwise, it stabilize to a lower value, which means that the fractions are no longer reacting.
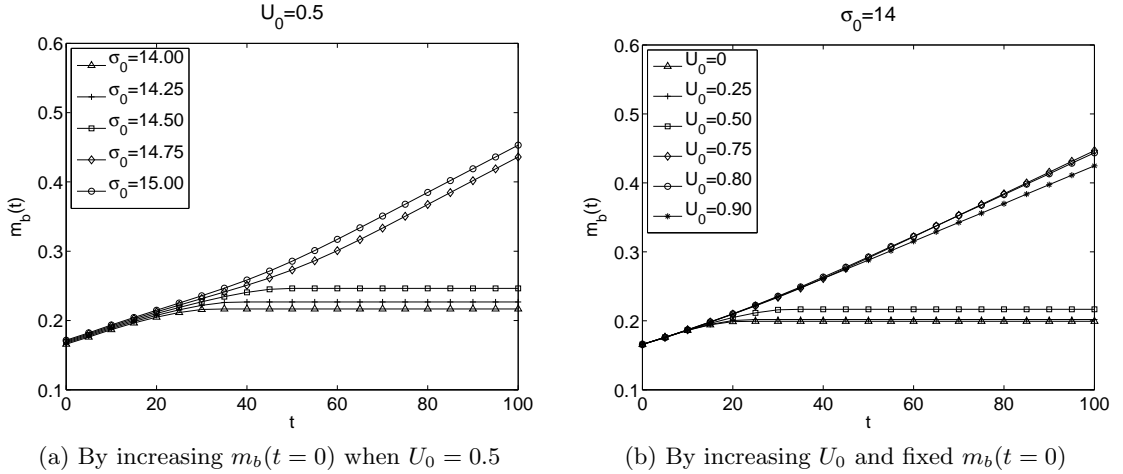

(a) By increasing $m_b(t = 0)$ when $U_0 = 0.5$ (b) By increasing U_0 and fixed $m_b(t = 0)$

FIG. **4.** Mass of burnt gas (m_b) as function of time. The ignition rate of reaction with threshold $c_s = 0.7$ is considered. Parameter values : $\alpha_2 = \frac{0.1}{(1-c_s)^2} = 1.111$ and the diffusion coefficient $\rho D = 0.4$.

We set up an initial condition as in (14) and we have varied σ_0, having fixed $U_0 = 0.5$, until the blow-off phenomena ocurr. Results are shown in Fig. 4 which confirms that, in the case of relatively high diffusion and slow reactions, if the initial burnt fraction is too low the reaction can quench. Then, if we fix the initial burnt fraction, Fig. 4 shows that by increasing the compressibility of the flow field (increasing U_0) the blow-off phenomena can disappear. In paricular, there is a maxium value of $U_0 \in [0.75, 0.8]$, for which the reaction quenchs with more difficulty. We have then studied the possibility of blow-off when the m$^{\text{th}}$ order Fisher's reaction is applied. The approach has been the same, so that we firstly fixed $U_0 = 0.5$ studying a range of σ_0 for which the blow off appears and than we fixed σ_0 studying the effects of compressibility. The rection never blows off as shown in Fig. 5.
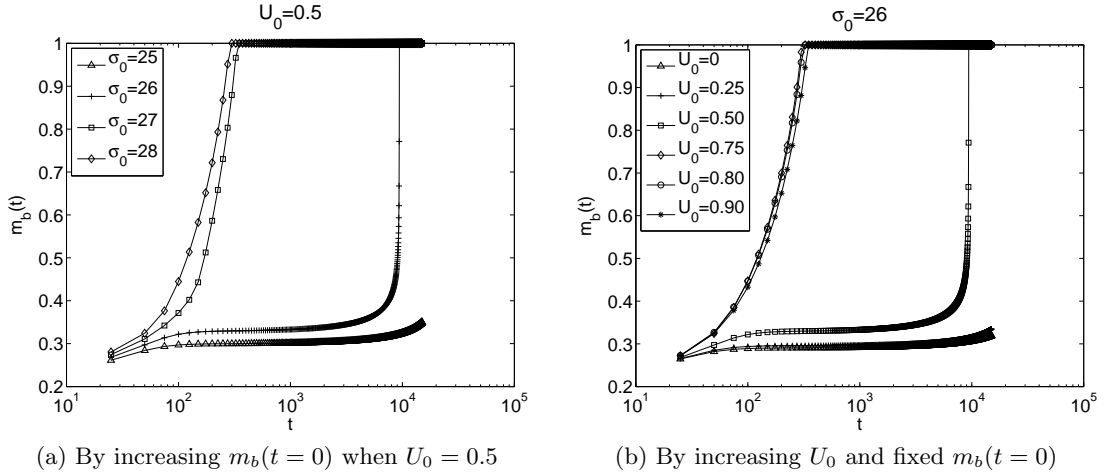
(a) By increasing $m_b(t = 0)$ when $U_0 = 0.5$ (b) By increasing U_0 and fixed $m_b(t = 0)$

FIG. **5.** Mass of burnt gas (m_b) as function of time. The general mth order with $m = 10$ reaction is considered. The parameter α_3 is such as $max[f_2(c)] = max[f_3(c)]$ and $\rho D = 0.4$.

4   Conclusion

This brief analysis has helped us to shed some light to the possibility of extending the models, typically used on the study of population dynamics, to the simplified advection-reaction and diffusion of the products of a combustion. In particular we showed that equation 6 applied to compressible flow fields leads to peaks of the concentration θ greater then unity. This means that, unless we rescale correctly the reaction term, the rate of reaction can take negative values. Since combustion is an irreversible process a suitable reaction term has to be positive or at least zero. We also studied the blow off phenomena which is typical for the ignition like reactions. We highlight then the role of compressibility of the flow field noting that by increasing the parameter U_0, as long as lower than 0.8, the efficiency of the reaction increases. At last, we have studied the blow off phenomena when general mth order Fisher reaction was applied. For these kind of reactions this phenomena does not occur because even for very low concentration of the combustion products the reaction rate is still greater then zero.

Références

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