Powder ignition modelling in interior ballistic problem

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1 Ignition in interior ballistic problem

Because of complex phenomena occurring, the modelling of interior ballistic flows is very difficult. The particular conditions of experiments (high pressure and temperature for example) do not give sufficient information to build rigorous models. Several correlations are used in internal ballistic codes, but they are often established in very different conditions. We focus our study on the powder ignition criteria, among the roughest approximation used in the ballistic community.

The most spread ignition criteria is summarized in two points

1. the surface temperature T_s of a grain is computed as an external heat flux is applied ;
2. when T_s reaches an empirically determined ignition temperature T_i, the grain is ignited and begins to burn (mass and energy transfer occur from the solid phase to the gas phase, nurning rate following the Vieille's law [12]).

The problem comes from the determination of T_i. It is considered as constant and measured with a "flat hot plate" method. It is well known that ignition temperature of energetic material depends on many parameters such as heat flux intensity or initial temperature. These dependencies are not taken into account by a so simple criteria.

Thus our work consists in developing a more complex model, based on physical considerations, which can reproduce some experimental phenomena. The only constraint, but not the least, is a low cost computation time. Actually, this model will be included into a new internal ballistic code (development in progress).

First we try to find an approximation of the unsteady heat equation in the solid phase, in order to simulate the heating of a grain. Then an ignition criteria developed by Lengellé [1] is adapted to our case. The last part deals with the introduction of chemical kinetic in the model, inspired by [4], in order to model the combustion in a low pressure range where Vieille's law is not valid.

At this point, we present some results that show the good behaviour of the complete model. Simulations are made with conventionnal thermodynamical datas found in literature. No comparisons with experiments have been done yet, due to the difficulty to obtain kinetic parameters of powders.

2 Unsteady powder heating

During ignition process of propulsive charges, a powder bed is exposed to a hot gas stream, escaping from a perforated tube (called igniter) with variable temperature and velocity. Figure 1 illustrates geometry around the interface of a grain.

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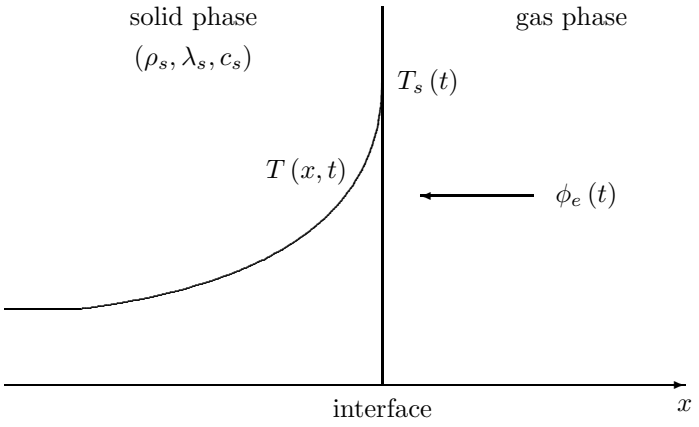


Figure 1: 1D interface configuration

ρ_s, λ_s and c_s respectively define the density, thermal conductivity and the heat capacity of the solid phase, and $\phi_e(t)$ is the convective heat transfer. The gas temperature will be noted T_g, with $T_g \geq T_s$.

In order to simulate the rise of the solid temperature, we have to solve the unsteady heat equation

$$\rho_s\, c_s\, \partial_t T + \lambda_s\, \Delta T = 0\,, \tag{1}$$

with the following initial and boundary conditions

$$T(x,0) = T_0, \quad T(+\infty, t) = T_0, \quad T\left(0^+, t\right) = T_s(t)\,, \quad E_{st}|_{0^+} = E_{in}|_{0^+} + E_g|_{0^+} \tag{2}$$

where x and t are the space and time variables, T_0 is the initial temperature, E_{st}, E_{in} and E_g are respectively the stored, received and generated energy.

Some analytical solutions under some geometrical assumptions can be found [8], using series development, but computations are not efficient. A Finite Difference (FD) algorithm can not be used considering its heaviness although it gives good results in general cases. By building assumptions on the temperature profile (parabolic [10] in AMI code or cubic [11] in MOBIDIC code) lead to an ODE. The loss of precision is compensated by the lightness of the method. We propose to consider an exponential profile such as

$$T(x,t) = a(t) + b(t) \exp\left(-\frac{r}{c(t)}\right) \tag{3}$$

where a, b and c are functions of t. Only one non linear equation has to be solved (by an iterative method).

3 Ignition criteria

Here we consider a 0^{th} order solid decomposition reaction [2] given by

$$\omega_s(x,t) = \rho_s\, A_s\, \exp\left(-\frac{E_s}{RT}\right) \tag{4}$$

with ω_s the reaction rate, A_s the pre exponential factor, E_s the activation energy and R the perfect gas constant. We adapt the idea proposed in [1]. Ignition occurs when the energy produced by the reaction

$\omega_s\, Q_s$ (Q_s heat of explosion) becomes non negligible compared to the energy received from the exterior. Thus, the ignition criteria can be expressed as

$$\int_0^e \rho_s\, Q_s\, A_s\, \exp\left(-E_s/RT\right)\, dx \geq \alpha \int_0^e \rho_s\, c_s\, \partial_t T\, dx\,, \tag{5}$$

where α is a fraction of energy (usually taken equal to 0.15 for composite propellants). e is an reactive thickness computed by

$$\frac{\omega_s\left(e,t\right)}{\omega_s\left(0^+,t\right)} = \frac{1}{10}\,. \tag{6}$$

4 Introduction of chemical kinetic in the gas phase

By introducing chemical kinetic, we intend to simulate burning rate at low pressure (out of pressure application's domain of Vieille's law [12]). We consider that chemical reactions in gas phase are almost steady. New configuration is illustrated in figure 2.

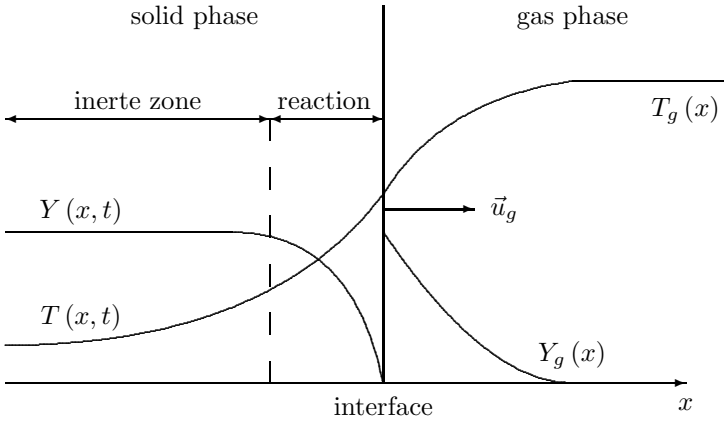


Figure 2: Introduction of chemical kinetic

Some simplifying hypothesis are made: very thin reaction zone in solid phase, only unimolecular reactions, 2^{nd} order reaction in the gas phase ([5], [6]), Lewis number equal to 1 and thick flame model (activation energy for gas phase reaction infinitely small [3], [7]).

The gas temperature T_g and the reactive species volumic fraction Y_g are expressed by

$$\lambda_g\, \Delta T_g - \rho_g\, u_g\, c_g\, \frac{d\,T_g}{d\,x} + \omega_g\, Q_g \;=\; 0 \tag{7}$$

$$\frac{\lambda_g}{c_g\, Le}\Delta Y_g - \rho_g\, u_g\, \frac{d\,Y_g}{d\,x} - \omega_g \;=\; 0 \tag{8}$$

where the reaction rate ω_g is expressed by

$$\omega_g\left(x\right) = A_g\, Y_g\, P^a \exp\left(-\frac{E_g}{R\,T_g}\right) \tag{9}$$

for a reaction of order a, where we note P the gas pressure, A_g the pre exponential factor, E_g the activation energy, λ_g the thermal conductivity, c_g the specific heat, ρ_g the density, u_g the gas velocity and Le the Lewis number. Boundary conditions are given by mass balance and energy balance.

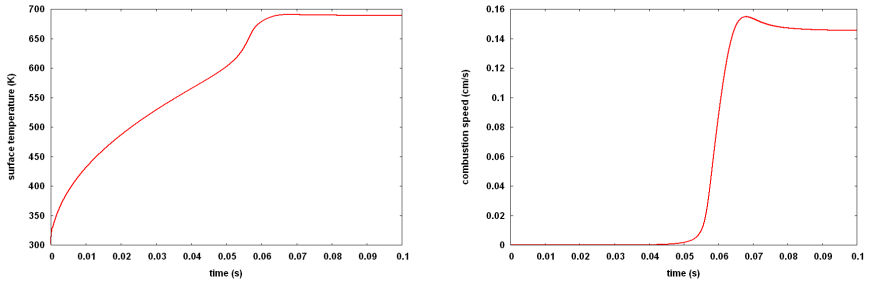
5 First tests

- Table 1 summarizes simulations and experimental results [1] concerning a propellant exposed to a CO_2 laser. We find a good agreement between results. We are aware that radiative and convective heat transfers are very different, but here we only want to show that our model reacts in a logical way : variable ignition temperatures and delay times depending on the external heat flux.

ϕ_e $(kW.m^{-2})$	t_{ign} exp (s)	t_{ign} sim (s)	T_{ign} sim (K)
4186.8	0.0022	0.0020	591
891.8	0.034	0.033	545
456.4	0.115	0.111	528
418.7	0.132	0.129	525
184.2	0.55	0.55	505
41.9	7.6	7.8	472

Table 1: Comparison simulations/experiments

- Combustion rate and surface temperature evolution obtained by coupling the equations of both phases are displayed in figure 3. At constant ambiant conditions, stationnary state appears.



a - Surface temperature evolution b - Combustion rate evolution

Figure 3: Simulations for a constant heat flux and ambiant pressure

- The external heat flux is now turned off at different moments. One can see on the figure 4 that after a certain time, even if there is no more external heating, steady combustion remains.

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- To finish, we demonstrate the compatibility of the model with the Vieille's law. Figure 5 shows that the steady combustion rate given by our model for low pressures (blue line) can be connected to a Vieille's law (green straight line). Here, if we express the Vieille's law as $r = u_g = u_s = a\,P^n$, we find $n = 0.89$ and $a = 1.445 \cdot 10^{-9}$. Such values are common in ballistic problems.

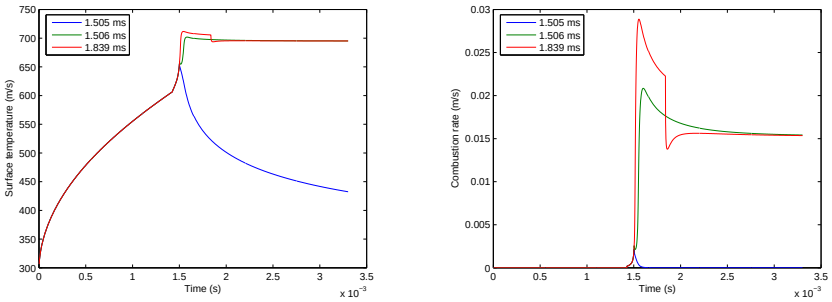

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Figure 4: Simulations with extinction of the external heat flux

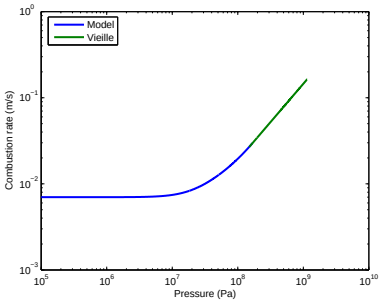

Figure 5: Combustion rate in function of ambiant pressure

6 Intermediate conclusion and perspectives

First results are very encouraging. The model react as expected when we modify parameters. Further development will be done with a more accurate description of the heat transfers. Characterization of the powders datas is in progress. Validations with experiments are planned as early as all datas are known.

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Annex : datas used for simulations

ρ_s	density	$1.6 \cdot 10^6\,\text{g.m}^{-3}$
c_p	heat capacity	$1.25604\,\text{J.g}^{-1}\text{.K}^{-1}$
λ_s	thermal conductivity	$16.077 \cdot 10^{-2}\,\text{J.m}^{-1}\text{.s}^{-1}\text{.K}^{-1}$
A_s	pre exponential factor	$1 \cdot 10^{17}\,\text{s}^{-1}$
E_s	activation energy	$168.569\,\text{kJ.mol}^{-1}$
Q_s	chemical heat released	$175.846\,\text{J.g}^{-1}$
λ_g	thermal conductivity	$8.37 \cdot 10^{-4}\,\text{J.m}^{-1}\text{.s}^{-1}\text{.K}^{-1}$
A_g	pre exponential factor	$2.36 \cdot 10^{-5}\,\text{g.m}^{-3}\text{.s}^{-1}\text{.Pa}^{-2}$
E_g	activation energy	$0\,\text{kJ.mol}^{-1}$
Q_g	chemical heat released	$2336.23\,\text{J.g}^{-1}$
M_g	molar mass	$24\,\text{g.mol}^{-1}$
r_0	radius of the grain	$5.715 \cdot 10^{-3}\,\text{m}$
T_0	initial temperature	$300\,\text{K}$