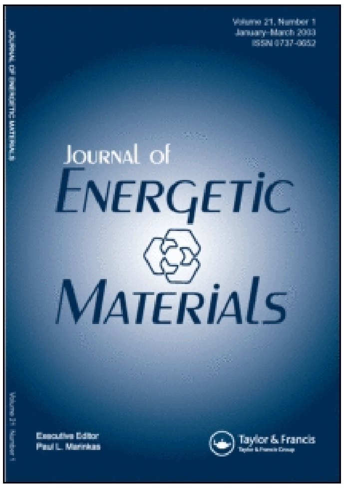

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Modeling of Closed-Vessel Experiments and Ballistic Parameter Estimation

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Closed vessels have been used for the regression of lumped ballistic parameters for decades. If material and energy balances are coupled with burning rate empirical correlations, uncorrelated parameters can be adjusted, describing accurately the thermochemical behavior of the generated gases, even if the chemical composition of the propellant

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is unknown (aging of the propellant). This work presents a system of differential equations integrated to produce pressure profiles within the vessel that are highly dependent on the choice of empirical parameters. Such parameters are manipulated via maximum likelihood statistical procedures, leading to the best set of parameters to describe the propellant.

Keywords: propellant, modeling, ballistic parameters estimation, closed vessel, energy and material balances

Introduction

Closed vessels traditionally have been employed in ballistics studies for the last six decades. They were mostly used for the estimation of bulk or lumped parameters commonly known as force, quickness, covolume, impetus, maximum pressure achieved, etc. Additionally, they have been employed as a quality control tool, providing information whether the propellant under testing is adequate for utilization or must be reprocessed.

However, for the design and simulation of gun performance, it would be rather important if one could use the thousands of P versus t points generated by a single shot for the estimation of as many ballistic parameters as possible.

Some of these parameters can also be evaluated through thermochemical calculations as in the well-known Hirschfelder-Sherman method [1]. However, this approach has the disadvantages of requiring an accurate chemical description of the propellant and of being predictive, rather than using experimental data on pressure profiles to improve its quality. In addition, aging of the propellant continuously changes its composition, which then must be monitored constantly.

The present work is devoted to the development of detailed energy and mass balances inside the closed vessel. These balances are coupled with several empirical models, and the model built this way has its performance compared to real experimental data, using known regression procedures (maximum likelihood in this case).

Mathematical Modeling

In the modeling, two main hypotheses were assumed:

a. There is no heat exchange between the system and the environment, once the burning time is negligible compared to typical heat transfer rates.
b. Inside the vessel an exothermic decomposition reaction takes place and can be represented by

$$\text{Solid} \rightarrow \text{Gas} + \text{Heat}. \tag{1}$$

The second hypothesis is due to the fact that one is not able to calculate (or is not interested in calculating) the chemical composition of the gas generated by the reaction but is, instead, devoted to predicting its thermochemical behavior and its formation kinetics.

The first law of thermodynamics [2] states that

$$dQ = dU + dW, \tag{2}$$

where dQ is the heat exchanged with the environment, dW is the amount of work performed, and dU is the increase in internal energy. Here and henceforth, every physical quantity will be assumed to be expressed in its correspondent SI unit (Système International d'Unités).

Once we assumed that no heat is exchanged (hypothesis a) and the vessel is rigid, then

$$dQ = 0 \quad \text{and} \quad dW = 0 \rightarrow dU = 0. \tag{3}$$

So by Equation (2) one can see that the energy envelope of the system is closed, which means that the total amount of energy is constant. Thus, initial energy is constantly distributed between the solid phase (subscript s) and the gas phase (subscript g):

$$\frac{dU_s}{dt} + \frac{dU_g}{dt} = 0, \tag{4}$$

where U_s is the energy of the solid and U_g is the energy of the gas.

Once the only experimental information available (besides P versus t data) is related to the heat of combustion at constant pressure, enthalpy is defined in the usual way [2]:

$$H = U + P \cdot V, \tag{5}$$

where P is the pressure and V is the volume. Time differentiation leads to

$$\frac{dU}{dt} = \frac{dH}{dt} \; P\frac{dV}{dt} \; V\frac{dP}{dt}. \tag{6}$$

The time derivative of enthalpy for each subsystem (solid and gas) is given by [2]

$$\frac{dH}{dt} = Cp\frac{dT}{dt} + \left[V - T\left(\frac{\partial V}{\partial T}\right)_P\right]\frac{dP}{dt} + \bar{H}\frac{dm}{dt}, \tag{7}$$

where Cp is the isobaric heat capacity, T is temperature, $\bar{H}$ is the specific enthalpy, and m is the mass of each subsystem. Expressions (6) and (7) will be applied to both solid and gas phases.

Once the thermal expansion coefficient of the solid is small, it is assumed that

$$\left(\frac{\partial V_s}{\partial T}\right)_P = 0. \tag{8}$$

So, for the solid, Equation (7) becomes

$$\frac{dH_s}{dt} = Cp_s\frac{dT}{dt} + V_s\frac{dP}{dt} + \bar{H}_s\frac{dm_s}{dt}, \tag{9}$$

where entities were already defined and are here applied to the solid (s).

Equation (9) is substituted in Equation (6), leading to

$$\frac{dU_s}{dt} = \overline{Cp}_s \cdot m_s\frac{dT}{dt} + \bar{H}_s\frac{dm_s}{dt} - P\frac{1}{\rho_s}\frac{dm_s}{dt}, \tag{10}$$

where ρ_s is solid density and $\overline{Cp}_s$ its specific heat capacity.

Specific enthalpy on temperature T can be calculated from its reference value on 298 K ($\bar{H}_s^{298}$) [2]:

$$\bar{H}_s = \bar{H}_s^{298} + \int_{298}^{T} \overline{Cp}_s \, dT. \tag{11}$$

So Equation (10) becomes

$$\frac{dU_s}{dt} = \overline{Cp}_s \cdot m_s \frac{dT}{dt} - P \frac{1}{\rho_s} \frac{dm_s}{dt} + \left[\bar{H}_s^{298} + \int_{298}^{T} \overline{Cp}_s \, dT \right] \frac{dm_s}{dt}. \tag{12}$$

An analogous procedure for the gas phase leads to

$$\begin{aligned} \frac{dU_g}{dt} = {} & -T \left(\frac{\partial V_g}{\partial T} \right)_P \frac{dP}{dt} - P \frac{dV_g}{dt} + \left[\bar{H}_g^{298} + \int_{298}^{T} \overline{Cp}_g \, dT \right] \frac{dm_g}{dt} \\ & + \overline{Cp}_g \cdot m_g \frac{dT}{dt}, \end{aligned} \tag{13}$$

where, once again, quantities were already defined and are here applied to the gas.

It is a common procedure in ballistics to employ Abel's equation of state to describe gaseous P versus V versus T behavior [2,3]. This work will not be an exception:

$$P \left(\frac{V_g}{m_g} - \eta \right) = \frac{RT}{M}, \tag{14}$$

where $R = 8.32$ J/mol/K is the gas universal constant, M is the average molecular weight of the generated gas, and η is its covolume, the last two demanding an statistical fitting procedure.

So the derivative required in Equation (13) becomes

$$\left(\frac{\partial V_g}{\partial T} \right)_P = \frac{R \cdot m_g}{P \cdot M}. \tag{15}$$

For reasons related to the computational time demanded, it is desirable to minimize the amount of state variables when dynamically simulating the system. Thus, the pressure time derivative is expressed in terms of its correspondent variations of mass and temperature, using Equation (14):

$$\frac{dP}{dt} = \frac{RT}{(V_g - \eta m_g)} \frac{1}{M} \frac{dm_g}{dt} \left[\frac{m_g}{(V_g - \eta m_g)} \left(\frac{1}{\rho_s} - \eta \right) - 1 \right] + \frac{R m_g}{M(V_g - \eta m_g)} \frac{dT}{dt}. \tag{16}$$

Since the total mass (m_t) inside the vessel is constant,

$$m_t = m_g + m_s = \text{constant} \rightarrow \frac{dm_g}{d_t} = -\frac{dm_s}{dt}. \tag{17}$$

and since total volume (V_t) is also constant,

$$V_t = V_g + V_s = \text{constant} \rightarrow \frac{dV_g}{dt} = -\frac{dV_s}{dt}. \tag{18}$$

The reference (standard) heat of combustion can be easily measured in a Parr Bomb at 298 K and is recognized to be

$$\Delta \bar{H}^{298} = \bar{H}_g^{298} - \bar{H}_s^{298}. \tag{19}$$

So Equations (2)–(19) are gathered to form the heat balance of the system, written in terms in which the time dependence of temperature is described:

$$\frac{dT}{dt} = -\left[m_g \cdot \overline{Cp}_g + m_s \cdot \overline{Cp}_s + \frac{R^2 m_g^2 T}{P \cdot M^2 (\eta m_g - V_g)} \right]^{-1} \times \left\{ \int_{298}^{T} (\overline{Cp}_s - \overline{Cp}_g) dt - \Delta \bar{H}^{298} + \frac{(R \cdot T)^2 m_g}{P \cdot M^2 (\eta m_g - V_g)} \times \left[\frac{m_g (1/\rho_s - \eta)}{(V_g - \eta m_g)} - 1 \right] \right\} \frac{dm_s}{dt}. \tag{20}$$

Much more simply, the mass balance consists basically of the Vielle/Moraour/Saint-Robert empirical rule of decomposition [3], to be considered together with Equation (17):

$$\frac{dm_s}{dt} = -S \cdot D \cdot P^{\alpha}, \tag{21}$$

where S is the total burning area and D and α are empirical parameters to be adjusted.

Quite frequently, the solid burning area can be easily related to its mass on each instant. However, in cases where grain geometrical complexity turns this to a difficult task, one can use empirical form functions such as [3]

$$\frac{S}{S_0} = \left[1 - \frac{4n}{(1+n)^2}\frac{m_{s0} - m_s}{m_{s0}}\right]^{1/2}, \tag{22}$$

where S_0 and m_{s0} are, respectively, the initial burning area and the initial grain mass. Parameter n is the form factor, known for several grain geometries [3]. However, it can be included in the set parameters to be adjusted if desired or needed. However, it is preferably to adjust n before the thermokinetic regression, which can be done considering only geometric aspects.

It must be said at this point that D and α can be adjusted in Strand-Burner fixtures, but at least three shots must take place in the vessel for that. With the present approach, the thousands of measurements in only one shot are used to adjust them with low variance.

The last constitutive (empirical) model required is the one for specific heat capacity for both gas and solid phases. The traditional form was employed [2]:

$$\overline{Cp}_g = A_g + B_g \cdot T + \frac{C_g}{T^2} \quad \text{and} \quad \overline{Cp}_s = A_s + B_s \cdot T + \frac{C_s}{T^2}, \tag{23}$$

where A_g, B_g, C_g, A_s, B_s, and C_s are the last empirical parameters to be adjusted. It must be said that the accurate estimation of these important parameters have been neglected up to this time [1], and this is another contribution of the present work.

Since the model performance does not depend strongly on A_s, B_s, C_s, and ρ_s, they are assumed to be known (values corresponding to thermoplastic polymers are good assumptions), and only D, α, η, A_g, B_g, C_g, M, and n are fitted.

So, briefly, the dynamic system (20) + (21) describes the evolution of a confined deflagration of a powder in terms of m_s and T. All other quantities (e.g., P, S, V_s, m_g, V_g, etc.) can be calculated with or related to these two (using the adequate equation); this is carried out in every simulation time. Successive simulations are conducted (manipulating the empirical parameters D, α, η, A_g, B_g, C_g, M, and n), and the pressure profiles obtained are compared to the experimental ones, until an optimal set of parameters is found, following the maximum likelihood statistical criterion [4]. This is conducted by a standard multidimensional optimization technique [5].

Computational Simulation

To simulate the dynamic functioning of the closed vessel, one iterates on the vector (identified by a line underneath) described by (20) + (21), having T and m_s as the only state variables, t as the independent variable, and all the others playing their role as auxiliary variables:

$$\frac{d\underline{F}(t)}{dt} = \begin{bmatrix} \dfrac{dT}{dt} & \text{given by (20)} \\ \dfrac{dm_s}{dt} & \text{given by (21)} \end{bmatrix}, \quad \text{where } F(t) = \begin{bmatrix} T \\ m_s \end{bmatrix}. \tag{24}$$

Euler's method is employed to update the vector of state variables $\underline{F}(t)$ from t to $t + \Delta t$, where Δt is the incremental time step (small and preferably made equal to the inverse of the acquisition frequency of the experimental apparatus):

$$\underline{F}(t + \Delta t) = \underline{F}(t) + \frac{d\underline{F}(t)}{dt}\Delta t. \tag{25}$$

An algorithmic description of the entire method is given below.

Initialization

a. Enter initial conditions initial mass (m_{s0}), initial temperature (T_0), and initial pressure (P_0).

Table 1
Parameter regression results

Fitted parameter	Unit	Value
D	m/s	2.46×10^{-9}
α	—	1.1703
η	$\mathrm{m^3/kg}$	1.1646×10^{-3}
A_g	J/kg/K	715.2916
B_g	$\mathrm{J/kg/K^2}$	1.0214
C_g	J·K/kg	1.0264
M	kg/mol	0.0232

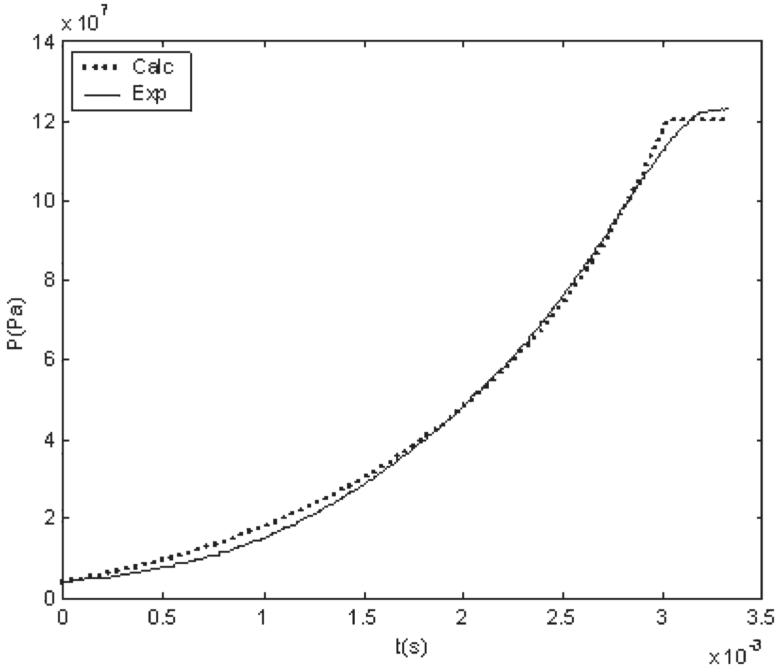

Figure 1. Results for load density $\Delta = 0.10\,\mathrm{g/ml}$.

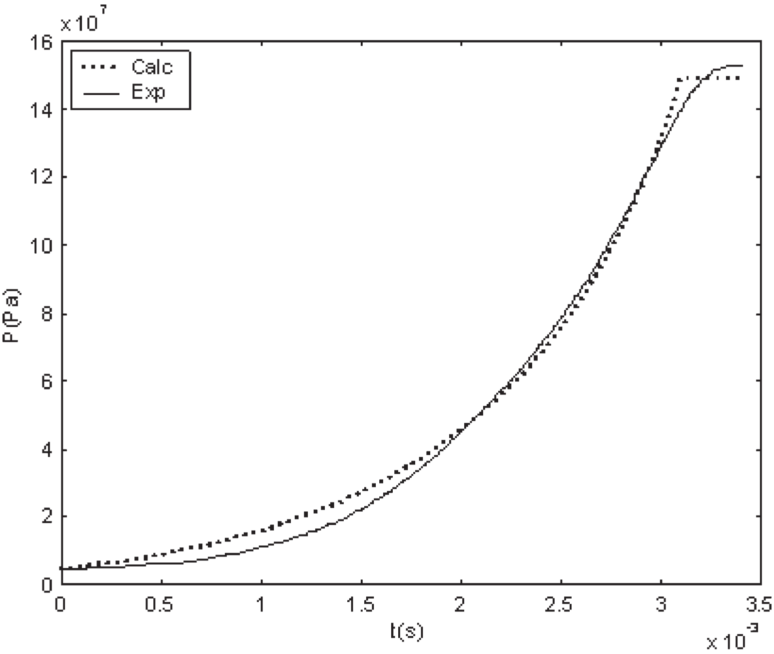

Figure 2. Results for load density $\Delta = 0.12\,\text{g/ml}$.

b. Enter vessel volume (Vt), grain dimensions (height, diameter, etc.), geometry (n), density (rhos), and heat of combustion ($\Delta\overline{H}^{298}$).
c. Enter estimatives for each empirical parameters (D, α, η, A_g, B_g, C_g, and M).
d. With (a) and (b), calculate the mass of each grain.
e. With (a) and (e), calculate the number of grains.
f. With (b) and (e), calculate the initial total burning area (S_0) and the initial total solid volume (V_{s0}).
g. With V_{s0} and Equation (18), calculate the initial total gas volume (V_{g0}).
h. With V_{g0} and Equation (14), calculate the initial total gas mass (m_{g0}).
i. With m_{g0} and m_{s0} and Equation (17), calculate the initial total mass (m_{t0}).

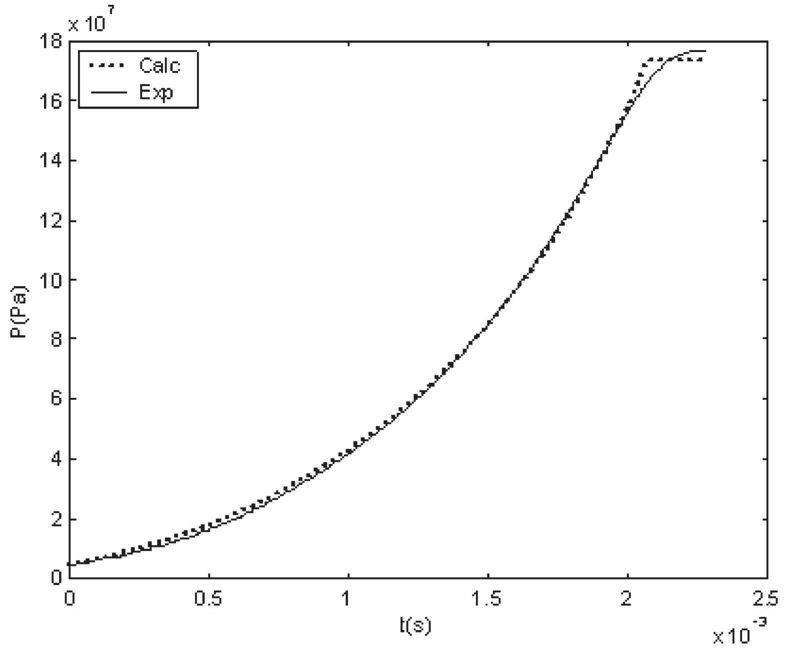

Figure 3. Results for load density $\Delta = 0.14\,\mathrm{g/ml}$.

Iteration (at Each Time Step Δt)

At each time t, there are available ancestor values for T and m_s, starting with $t = 0$, $T = T_0$, and $m_s = m_{s0}$. From t, to $t + \Delta t$,

a. Calculate the volume occupied by the solid ($V_s = m_s/\rho_s$).
b. Calculate the volume occupied by the gas ($V_g = V_t - V_s$).
c. Calculate the gas mass ($m_g = m_t - m_s$).
d. Calculate the pressure with Equation (14).
e. Calculate the burning area with Equation (22).
f. Calculate the time derivative of state variables with Equations (20) and (21).
g. Update the values for m_s and T with Equation (25).
h. Go to (a).

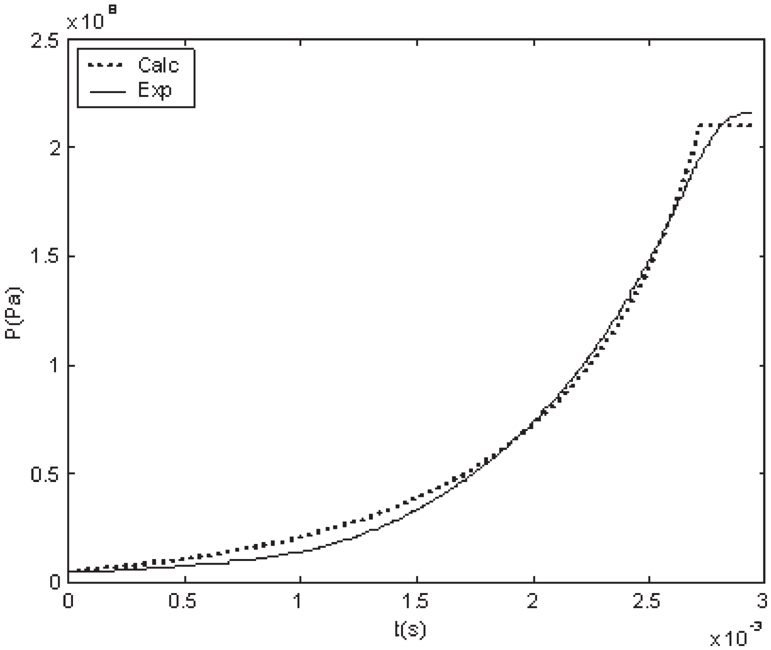

Figure 4. Results for load density $\Delta = 0.16\,\text{g/ml}$.

Parameter Estimation

A standard nonlinear parameter estimation procedure was employed to fit ballistic parameters D. α, η, A_g, B_g, C_g, and M. Once experimental data were based on P (henceforth called $\underline{P}^{\text{exp}}$) versus t information, the simulation was conducted using m_s and T as state variables, but the calculated pressure (generated within the algorithm), henceforth called $\underline{P}^{\text{teo}}$, was indeed used for regression purposes.

Based on the statistical criteria of maximum likelihood [4], a sum of weighted residuals is defined:

$$\Phi = (\underline{P}^{\text{teo}} - \underline{P}^{\text{exp}})^t \underline{W} (\underline{P}^{\text{teo}} - \underline{P}^{\text{exp}}), \tag{26}$$

where $\underline{W}$ is a variance-covariance matrix. Usually it is made equal to an identity matrix, and the minimum square procedure is recovered.

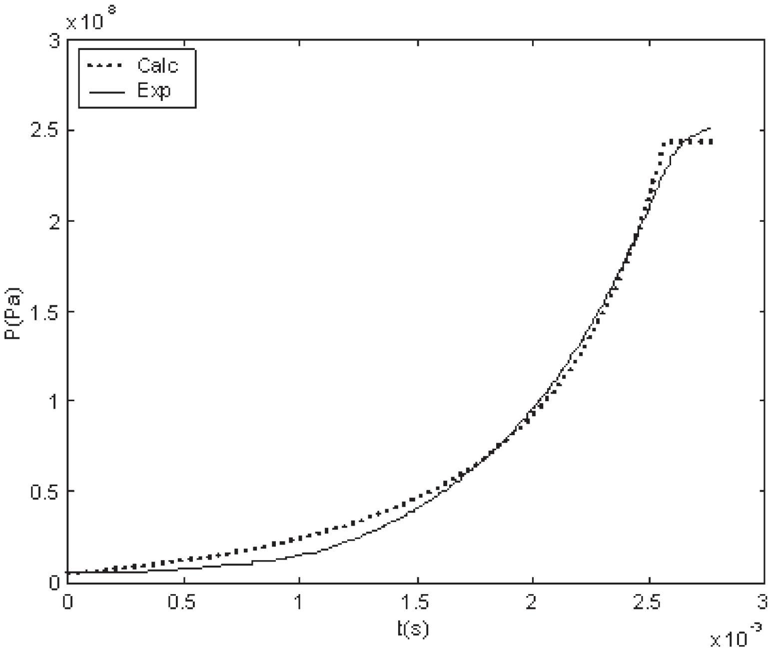

Figure 5. Results for load density $\Delta = 0.18\,\mathrm{g/ml}$.

As already mentioned, successive simulations are conducted, and ballistic parameters (D, α, η, A_g, B_g, C_g, and M) are changed during the process aimed at the minimization of Φ:

$$\overset{\text{Min}}{\left\{D, \alpha, A_g, B_g, C_g, M, n, \eta\right\}}\Phi. \tag{27}$$

This is conducted also by standard multidimensional optimization techniques; this work employed a Newton method, with a BFGS update of the Hessian matrix [5], which will not be considered in detail.

Results

A complete procedure was conducted, using several density loads ($\Delta = m_{s0}/Vt$) and a double-base powder in the form of small strips (length $= 0.1773\,\mathrm{m}$, width $= 0.015\,\mathrm{m}$, and

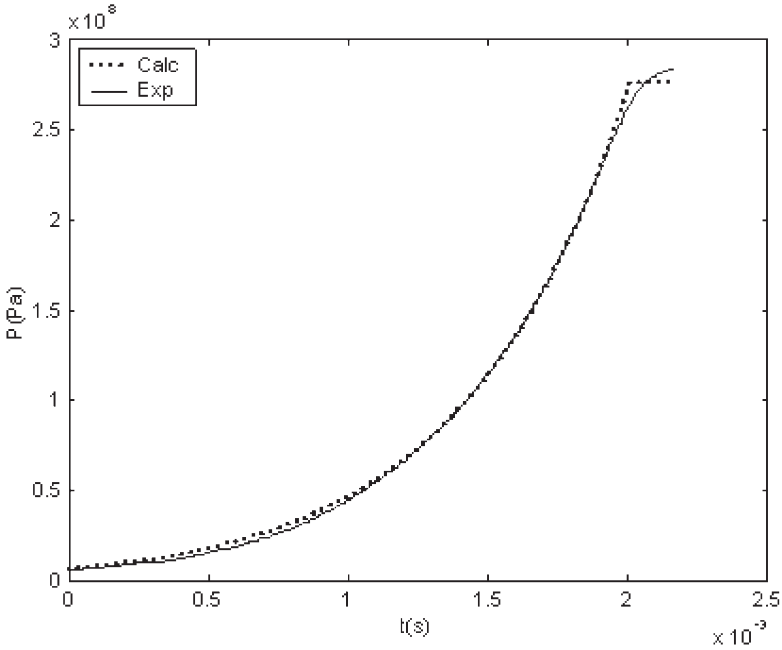

Figure 6. Results for load density $\Delta = 0.20\,\mathrm{g/ml}$.

thickness = 0.0004 mm, $n = 0$, $\Delta\overline{H}^{298} = 5{,}128{,}830\,\mathrm{J/kg}$). Results are reproduced in Table 1 and depicted in Figures 1–6.

Conclusions

With the set of tools developed here, it was possible to fit ballistic parameters D, α, η, A_g, B_g, C_g, and M, which define the thermo-chemical behavior of the powder and its kinetics of decomposition, even if the chemical composition of the propellant is no longer known (aging of propellant). This is important information for the design of devices that use such components (guns, howitzers, mortars, rockets), if design is conducted including rigorous energy balances (mainly because of A_g, B_g, and C_g estimations). On the other hand, it is also useful for simulations, if one is interested in predicting the behavior of the gun after propellant aging. Additionally, with the fitted model, it is possible to design the experimentation, fixing experimental coordinations (mainly load densities) to prevent overpressures and/or to obtain the maximum number of information with the minimum number of tests. Regression showed good adherence to experimental data (Figures 1–6) and numerical values of fitted parameters values are reasonable (Ag, Bg, Cg and M, for instance).

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