

EVOLUTIONARY ALGORITHMS FOR PROPELLANTS PARAMETERS IDENTIFICATION

Aleksander Górniak, Andrzej Kaźmierczak

Wroclaw University of Technology
Department of Motor Vehicles and Combustion Engines
Braci Gierymskich Street 164, 51-640 Wrocław
tel.: +48/(71) 347 79 26, fax +48/(71) 347 79 18
e-mail: aleksander.gorniak@pwr.wroc.pl, andrzej.kazmierczak@pwr.wroc.pl

Abstract

This paper presents the possibility of the parametric identification of an unknown low energy explosive basing only on its ballistic curve using advanced optimisation algorithm. What was under investigation here was the approach of an explosive replication for the numerical investigation of ANSYS AUTODYN solver. The emphasis was given here for the propellants used in the automotive safety devices. The results of closed bomb testing was compared with its numerical representation. The required parameters to develop a new numerical model of an explosive was identified with the aid of evolutionary algorithm. In order to perform a parametric identification a mathematical model of considered phenomenon is required. Hence, this paper contains a mathematical model of a deflagration process which was the basis for the evolutionary algorithm. The algorithm verified a variety of parameters until the objective function is obtained. In the case of this paper the objective function was a ballistic curve of an unknown explosive which combust under deflagration regime. The results obtained with this method shows good agreement with the closed bomb test of the propellant. Furthermore, advanced optimisation tools such as an evolutionary algorithms, in oppose to most of other optimisations algorithms, enables to find a global optimum. However, the identified function here was found to be unimodal.

Keywords: evolutionary algorithms, global identification, closed vessel test, propellants

1. Introduction

The characteristics of a propellants is determined during a closed vessel (bomb) tests. This test consists on firings a defined portion of a defined propellants in a closed volume with no movable barriers giving the pressure versus time (dp/dt) properties. This article presents a procedure for determining parameters of a propellants considering only the results of such a test. The closed bomb test was used for determination of a propellant burning properties. It was found that this method can be dependent on the type of ignition and it was mainly performed for the limited range of densities [1]. The parameters are determined with aid of an evolutionary algorithm.

The evolutionary algorithms is a method of global optimisation or identification. The difference between those terms is that optimisation is searching for an extremum of a function, while the parametric identification is searching the parameters of a known mathematical model in order to reproduce an objective function (e.g. as it is in the case of this paper, the ballistic curve).

Evolutionary algorithms search the space of alternatives solution looking for the optimal one, changing in every step a group of solutions to the problem. The evolutionary algorithms operates on a definitions similar to those used in natural studies. For example the particular solution is called an *individual*. *Population* is a group of solution of a considered problem (hence, population is a group of *individuals*). The *environment* is defined as a possible solution of a problem enclosed within assumed area of searching. Adaptation of individuals ("*fitness*") in the *population* is defined for a given task optimization objective function. Numerical evolution of *individuals* is similar to Darwin's theory of evolution. Therefore, a process of generational renewal in which the better individuals are more likely to transmit its genetic code. In the next iteration of the algorithm

more mutated copies of the parent *individuals* (i.e. *descendants*) were selected with probability proportional to their *fitness* [2], [3].

2. Mathematical model used for the parametric identification

The parametric identification requires a mathematical description of a considered phenomenon. In the case of this paper the emphasis is given for a deflagration process of a propellant. In general, propellants are explosives which combust under deflagration rather than detonation regime. The main difference between detonation and deflagration is the speed of the explosive burning. When the grain of an explosive combusts with speed greater than speed of sound then it is said that the material detonates and the pressure wave provoked by this is called detonation wave. The burning process slower than the speed of sound characterises deflagration and the pressure wave in this case is called a flame. The ANSYS AUTODYN solver is capable of simulating both kind of explosives (i.e. detonation and deflagration) although in oppose to the detonation the solvers library does not provide any deflagrating material [4]. However, the AUTODYN gives a possibility to create a numerical model of a propellant representing required quantities. It is done by entering appropriate parameters for the equation of state mathematically describing the deflagration phenomenon.

The deflagration in AUTODYN solver is simulated by the “*Powder Burn*” Equation of State. This includes recently implemented combustion models depended on the form of combusted material. Those implementation are:

- the JWL equation of state with constant burning rate,
- exponential equations of state characterised by the burning rate dependant on pressure.

According to [4] and [5] the “*Powder Burn*” model is multiphase model in which gas and solid particles exists in one cell at the same time. The total mass inside a cell is a sum of the mass of the gas and the mass of the unburned solid particles. The volume of both gas and the solid particles is known, hence the density, compression etc. are calculable.

AUTODYN recognises the combustion of an explosive as a function of reaction fraction given by (1) [4]-[6].

$$F(t) = \frac{M_s(t_0) - M_s(t)}{M_s(t_0)}, \quad (1)$$

where:

$F(t)$ – reaction fraction,

$M_s(t)$ – mass of burned material within the time of (t) . The initial time is denoted with indeks „0“.

The exponential equations of state, recently implemented to the ANSYS AUTODYN solver, is used to determine the gas pressure within the chamber (equation 2) which then can be utilised in equations (3) and (4) for burning rate determination.

$$p_g = \rho_g e_g e^{\left(\frac{\rho_g}{D}\right)}, \quad (2)$$

One of main parameters is a burn rate which describes the efficiency of a propellant. The burning rate is depended on pressure and temperature [7]. The linear dependency of a burning rate to pressure is expressed by equation (3).

$$r = r_1 p_g, \quad (3)$$

However, due to limitation to the validity of a linear approach to the burning rate [1], [8] the exponential form of the burning rate equation (known as Vieille’s law) is used [1], [7]-[9]:

$$r = \beta \cdot p_g^\alpha, \quad (4)$$

where: (equations (2), (3) and (4)):

r – burning rate,
 r_1 – constant for given type of the propellant,
 α – pressure index, function of a propellant composition,
 β – burning rate constant depending on the propellant initial temperature,
 p_g – gas pressure in a closed bomb chamber,
 e_g – internal energy,
 D – user defined constant.

As it was stated in publications referred under [1], 8-10] the burning rate of a propellant can be also determined on the base of differentiated smoothed, experimental time dependant pressure curve obtained during closed bomb test (equation 5):

$$r = \frac{de_w}{dt} = \frac{de}{dz} \cdot \frac{dz}{dp} \cdot \frac{dp}{dt}, \quad (5)$$

where:

e_w – thickness of burnt layer of the propellant,
 t – time,
 p – pressure,
 z – mass portion.

The thickness of burnt layer of the propellant is the only shape dependent factor in mathematical model of a propellant combustion. Assuming that all grains are the same shape, the influence of the shape of a propellant grain on its characteristics is described by equation (6).

$$\frac{de_w}{dz} = \frac{V_{z0}}{S_0} \frac{1}{\phi(z)}, \quad (6)$$

where:

$\frac{de_w}{dz}$ – the grain form function,
 V_{z0} – initial volume of the propellant grain,
 S_0 – initial surface of the propellant grain,
 $\phi(z)$ – form function (equation 7) :

$$\phi = \frac{S}{S_0}, \quad (7)$$

where:

S – surface of the propellant grain.

Algebraic form of ballistic curve $p(t)$ can be described by the differential equation of the mass fraction (z) of burnt material. The mass fraction is given by (8):

$$z = 1 - \frac{m}{m_0} = 1 - \frac{V_z}{V_{z0}}, \quad (8)$$

where m and V_z are the mass and volume of the propellant respectively. The subscript “0” denotes the initial stage (before ignition of the propellant) of said values [9].

The differential equations describing the dependence of the form of changes in mass fraction in relation to the pressure change is represented by the Noble-Abel equation of state (9).

$$\frac{dz}{dP} = \frac{1}{p_{max}} \frac{1 + \left(\eta_{exp} - \frac{1}{\rho_g} \right) \frac{p_{max}}{f_{exp}}}{\left(1 + \left(\eta_{exp} - \frac{1}{\rho_g} \right) \frac{p_g}{f_{exp}} \right)^2}, \quad (9)$$

where:

p_{max} – maximum pressure obtained during the closed vessel tests,
 η_{exp} – CO volume,
 ρ_g – gas density,
 f_{exp} – specific internal energy of the propellant.

3. The evolutionary algorithm set up

The evolutionary algorithm was set to determine the parameters of an explosive basing only on its ballistic curve. The mathematical model according to which the identification was performed was developed in order to satisfy the requirements of the “Powder Burn” Equation of State. Each individual presents 5 characteristics are presented in Tab. 1. Taking into consideration that only the ballistic curve is known here the environment is very large. Because of this the algorithm will present greater flexibility in searching the optimal value.

Tab. 1. The characteristics to be determined by the evolutionary algorithm

Characteristic	Symbol	Environment		Unit
		$\geq$	$\leq$	
Density of the solid propellant	ρ_s	100	4000	kg/m^3
Co volume	η_{exp}	10^{-4}	10	m^3/kg
Specific energy	f_{exp}	10^3	10^9	J/kg
Coefficient α	α	0.005	1.5	---
Coefficient β	β	0.005	1.5	---
Constant values				
Maximum pressure	p_{max}	33		MPa
Initial volume of solid propellant	V_{z0}	$1.90 \cdot 10^{-5}$		m^3
Initial value of solid propellant	S_0	$3.85 \cdot 10^{-5}$		m^2

It must be stated however, that there are simplifications assumed here which forbids the results to be considered identical to real. Those assumptions are listed below:

1. There is only one grain with smooth regular cylindrical shape with radius of 4 mm and height of 5mm.
2. All ignition systems and wires existing in real devices are disregarded here.
3. The housing of a propellant is disregarded.

For each individual the algorithm determines the fitness value which in this case is a mean-square error between the ballistic curve obtained experimentally and the ballistic curve numerically identified.

As it was already stated each individual has 5 characteristics (Tab. 1). The tests assumes reaching 10000 generations having 5 individuals in each population. The individuals representing the best fitness value was inherited. The inheritance was performed by means of the mutation operator while the selection operator was set to be a roulette selection. The stop criterion was reaching the final generation or finding the solution with the fitness value lower than 10^3 .

The calculation were performed in Matlab software. The block diagram representing mathematical model used for the parameter identification was design in Simulink (see Fig. 1). The algorithm changes the characteristics from Tab. 1 in order to find the α and β coefficients for the Vieille's law (equation 4). Those coefficients are constant so it is possible to assign appropriate burning rate to the gas pressure (p_g). The gas pressure in turn was found by means of closed bomb experiment. At this same time the algorithm adjusts the parameter shown in equation (3) until the identified ballistic curve is fitted to the one obtained experimentally.

4. Results and discussion

The results of the parametric identification are shown in Tab. 2. Values presented here are average of 50 runs of the algorithm due to the fact that in assumed environment, the identified function appears to be unimodal. Each time, before the algorithm was started, the generator seed of randomized values was engaged in order to ensure appropriate conduct of randomized trials.

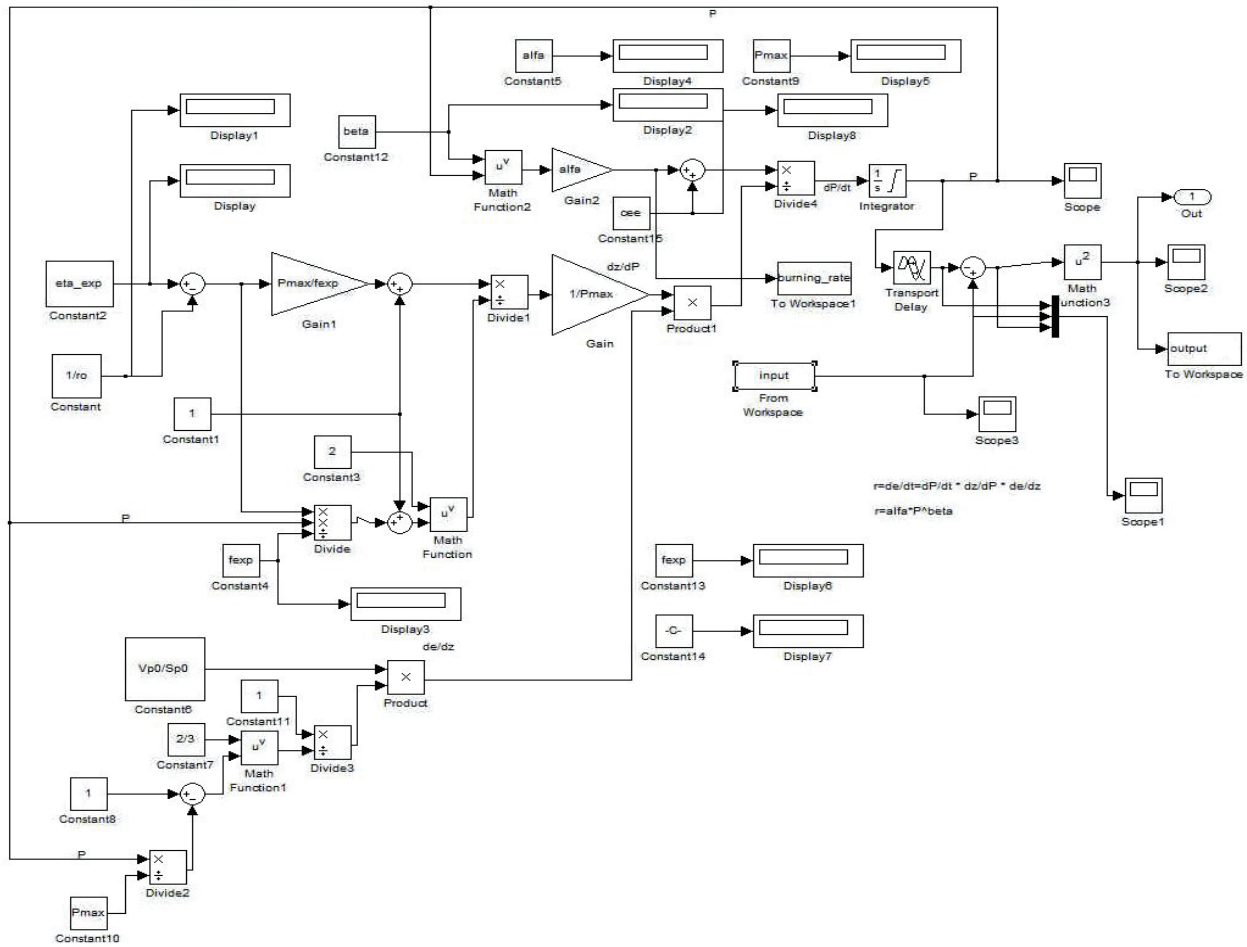


Fig. 1. The block diagram of a mathematical model for the parametric identification

Tab. 2. Results of the parametric identification

Characteristic	Symbol	Value	Unit
Density of the solid propellant	ρ_s	1206.23	kg/m^3
Covolume	η_{exp}	3.264E-04	m^3/kg
Specific energy	f_{exp}	9.40E+06	J/kg
Coefficient α	α	0.05	---
Coefficient β	β	0.59	---
Fitness	0.1090		

The results of parametric identification are presented on Fig. 2. Here the objective function is a ballistic curve obtained during the closed vessel tests. The identified with aid of the evolutionary algorithm curve shows reasonable good fitting with the objective function. It is proven by the value of the mean square error. The error on the beginning of the process (i.e. in the time range of 0 to 1 ms) deviates relatively strong comparing with the rest of the process. It is due to the refraction of the experimental ballistic curve. The algorithm endured difficulties in finding appropriate points and connecting it with a straight line. Hence, this error is rather originated by insufficient reproduction of the objective function obtained during closed vessel tests.

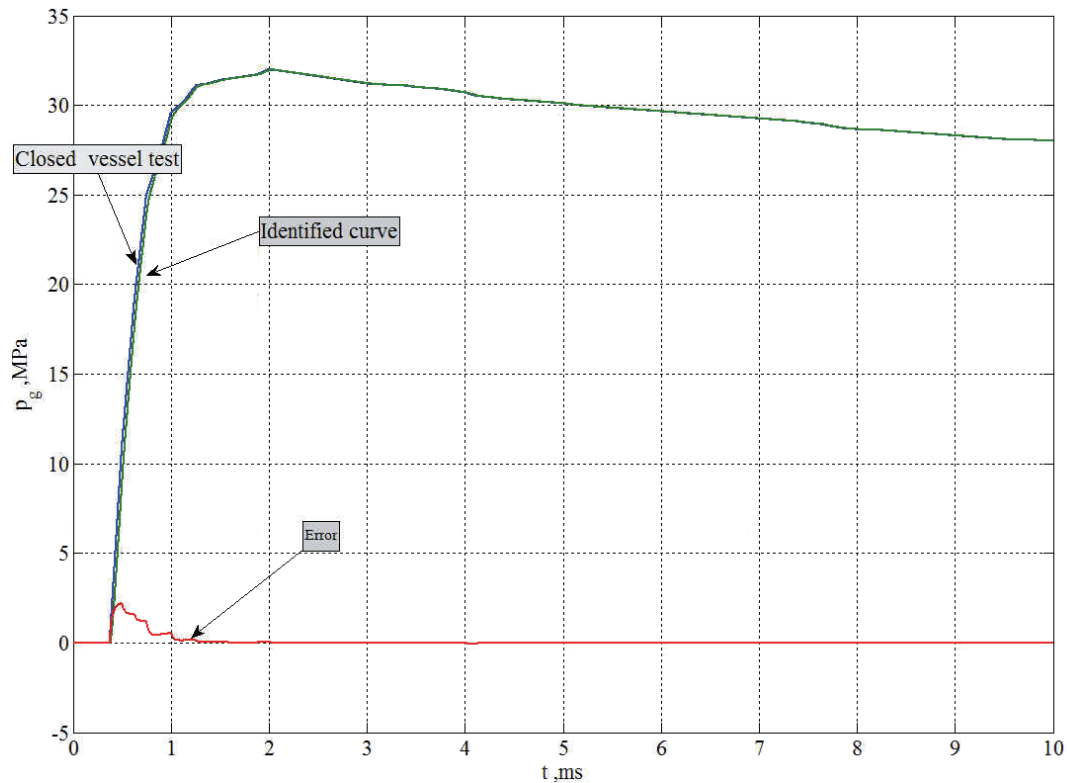


Fig. 2. The results of the parametric identification

5. Conclusion

What was presented here was the possibility to identify parameters of an unknown propellant basing only on its characteristic. Those parameters were found with aid of advanced optimisation tool (i.e. evolutionary algorithms). This method shows the most accurate results comparing with other optimisation methods (Monte Carlo method or least squares method). Furthermore, evolutionary algorithms are very easy to program and control.

The parametric identification presented here is subjected to simplification which forbids the parameters to be considered as real. Moreover, due to the lack of information about the propellant material (e.g. its chemical composition) it was impossible to compare obtained values. However, it should be stated that those parameters have been identified in terms of the development of a new numerical model of an explosive. Such a simplification significantly reduced the time of computation without affecting the accuracy of results. Nevertheless the method presented here, when enriched with more accurate mathematical model, can be used for very accurate identification of an unknown propellant. This however, requires greater computation power and longer time to perform accurate tests.

References

- [1] Liciejewski, Z. K., Surma, Z., *Effect of Application of Various Ignition Conditions in Closed-Vessel Tests on Burning Rate Calculation of a Fine-Grained Propellant*, Combustion, Explosion, and Shock Waves, Vol. 47, No. 2, pp. 209-216, 2011.
- [2] Arabas, J., *Wykłady z algorytmów ewolucyjnych*, WNT, Warszawa 2001.
- [3] Lis, J., *Parametryczno-nieparametryczna identyfikacja złożonego układu napędowego z silnikiem indukcyjnym*, Rozprawa doktorska, Politechnika Wrocławska, 2008.
- [4] Introduction to ANSYS AUTODYN, Material models, Chapter 9, ANSYS, Inc.
- [5] ANSYS, Inc. ANSYS AUTODYN User's Manual, Release 14.5 October 2012.

- [6] Atwood, A., Friis, E. K., Moxnes, J. F., *A Mathematical Model for Combustion of Energetic Powder Materials. 34th International Annual Conference of ICT*, Karlsruhe Federal Republic of Germany, June 24-27, 2003.
- [7] Agrawak, J. P., *High energy materials, Propellants, Explosives and Pyrotechnics*, WILEY-VCH, 2010.
- [8] Liciejewski, Z. K., *Experimental Study of Possibilities for Employment of Linear Form of Burning Rate Law to Characterise the Burning Process of Fine-Grained Propellants*, Central European Journal of Energetic Materials, 5(1), pp. 45-61, 2008.
- [9] Jeunieu, L., Lefebvre, M. H., Papy, A., Pirlot, M. C., *Guillaume P., Influence of the size distribution on the combustion rate of a spherical propellant*, 20th International Symposium on Ballistics, 2002.
- [10] Liciejewski, Z. K., *Influence of ignition method and loading conditions in closed vessel test on the burning rate of a propelling charge*, High Energy Materials, Vol. 1, pp. 152-160, 2009.

