# Treatment of Deterred Propellants in Interior Ballistic Calculations

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*In the paper the procedure for determination of deterred propellant characteristics that are necessary as input parameters in interior ballistic calculations is given. The basic features of developed model for interior ballistic cycle calculation of systems with deterred propellant propelling charge are presented. The model verification is carried out through comparison of computational results with American experimental data of 20 mm rounds with ball propellant propelling charge.*

***Keywords:*** *interior ballistics, propellant, propelling charge, deterrent.*

## 1. INTRODUCTION

In modern interior ballistic practice it is often required to design such a propelling charge that will provide practically maximum performance to the given gun-projectile system. The character of existing limitations usually imposes the requirement for very high progressivity of propellant combustion.

The possibilities are limited to obtain specific favourable rate of propellant gas formation during interior ballistic cycle only by the variation of propellant grain geometry. Therefore, the required combustion progressivity if often provided by the use of chemically modified (deterred) propellants.

The existing interior ballistic models are incapable to treat adequately the combustion of deterred propellants. Therefore, these models are practically useless in many cases where sophisticated design of high performance propelling charge is required. That is why the new interior ballistic model is developed for propelling charges composed of deterred propellants. The main particularities of the developed model will be presented here; the special attention will be paid to the specific case of ball propellants combustion. The procedure for determination of deterred propellant characteristics, which are necessary as input parameters for interior ballistic calculations, will also be considered.

The penetration depth of deterrent, its chemical identity, and its concentration level in the propellant characterise the deterred region from the chemical point of view for purposes of interior ballistic calculations. The reason that the penetration depth and the concentration of deterrent in the total propellant composition are considered sufficient to chemically characterise the deterred layer is due to the special shape of the concentration profile of the deterrent in propellant grains.

## 2. CHARACTERISTICS OF DETERRED PROPELLANTS

The deterrent concentration profile has been experimentally determined. The concentration profile shape for the case of dibutyl phthalate (DBP) penetration in the ball propellant grain is presented in Figure 1 [1].

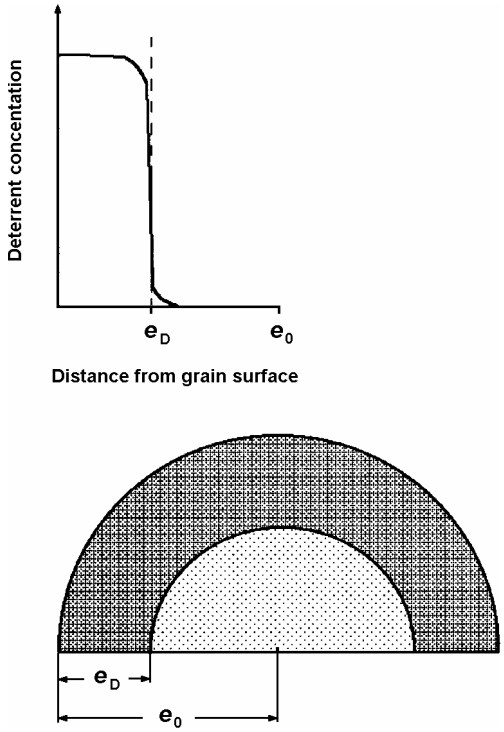


**Figure 1. Deterrent concentration profile in the spherical propellant grain**

The figure shows the shape of a diffusion front of a given plastisizer into a polymer matrix. This shape indicates that the deterrent concentration is nearly constant in the deterred layer and decreases sharply at the boundary line between deterred and undeterred regions. The consequence of a square-wave deterrent concentration profile is that one can assume a constant level of deterrent in the deterred region and that all of the deterrent in the propellant is evenly distributed through the deterred region (step function). The mean penetration depth of deterrent $e_D$ is a mean distance from the propellant grain surface to the boundary between the deterred region and the grain interior where there is almost no deterrent.

In the case of propellants with nonuniform particle size, such as ball propellants, the propellant granulation must be known to make possible the determination of the mass fraction of propellant grain deterred layer.

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The granulation of WC 870 (lot A.L. 45137) unrolled ball propellant is given in Table 1, where $\phi_i$ is the propellant mass fraction retained at $i$-th sieve and $d_i$ is the $i$-th sieve hole diameter.

**Table 1. Granulation of WC 870 (lot A.L. 45137) propellant**

| Sieve No. | $\phi_i$ | $d_i$ [mm] | $d_{m,i}$ [mm] |
|---|---|---|---|
| U.S. # 16 | 0.0000 | 1.197 | |
| # 18 | 0.0324 | 1.003 | 1.100 |
| # 20 | 0.3275 | 0.841 | 0.922 |
| # 25 | 0.5214 | 0.707 | 0.774 |
| # 30 | 0.1051 | 0.595 | 0.651 |
| # 35 | 0.0102 | 0.500 | 0.548 |
| # 40 | 0.0021 | 0.420 | 0.460 |
| PAN | 0.0094 | 0.354 | 0.387 |

In the case of constant propellant density (nitroglycerine is assumed to be uniformly distributed throughout the grain) the deterred layer mass fraction of unrolled ball propellant is defined by the following expression:

$$M_D = 1 - \frac{\phi_1\left(d_1 - 2e_D\right)^3 + \sum_{i=2}^{n-1}\phi_i\left(d_{m,i} - 2e_D\right)^3 + \phi_n\left(d_n - 2e_D\right)^3}{\phi_1 d_1^3 + \sum_{i=2}^{n-1}\phi_i d_{m,i}^3 + \phi_n d_n^3} \quad (1)$$

where $d_{m,i} = (d_i + d_{i-1})/2$ and $\phi_n$ is the propellant mass fraction passed through the finest sieve.

The assumption of constant propellant grain density represents certain deviation from real conditions. However, this assumption is fully acceptable in interior ballistic calculations.

For given WC 870 propellant granulation and measured mean deterrent penetration depth $e_D = 0.056$ mm the deterred layer mass fraction $M_D = 0.3621$ is obtained.

When propellant chemical composition is known, the $i$-th component mass fraction in undeterred layer of propellant grain ($X_i$) is given by the following expression:

$$X_i = S_i \cdot \frac{1}{1 - S_D} \quad (2)$$

where $S_i$ is the $i$-th component mass fraction in the propellant and $S_D$ is deterrent mass fraction in the propellant.

The deterred layer of propellant grain contains all the deterrent, and consequently the deterrent mass fraction in this region is:

$$Y_D = \frac{S_D}{M_D}. \quad (3)$$

The mass fractions of other components in deterred layer are proportionate to the mass fractions of corresponding components in undeterred layer of propellant grain. So, the $i$-th component mass fraction in deterred layer is:

$$Y_i = X_i \cdot \left(1 - S_D\right). \quad (4)$$

The chemical composition of WC 870 (lot A.L. 45137) spherical ball propellant is given in the left column of Table 2. The moisture (water) and residual solvent (ethyl acetate) have been arbitrarily taken to be equal to one-half of the total volatiles (1.26 %). The compositions of deterrent-containing and undeterred regions calculated by (2), (3) and (4) are presented in the middle and right column of Table 2.

**Table 2. Overall chemical composition of WC 870 (lot A.L. 45137) propellant with deterred and undeterred layers composition**

| Ingredient | Overall composition [%] | Deterred layer [%] | Undeterred layer [%] |
|---|---|---|---|
| Nitrocellulose (% of nitrogen) | 79.70 (13.11) | 71.89 (13.11) | 84.13 (13.11) |
| Nitroglycerine | 9.21 | 8.31 | 9.72 |
| Dibutyl phthalate | 5.27 | 14.55 | 0.00 |
| Dinitrotoluene | 0.64 | 0.58 | 0.68 |
| Diphenylamine | 0.88 | 0.79 | 0.93 |
| Water | 0.63 | 0.57 | 0.67 |
| Ethyl acetate | 0.63 | 0.57 | 0.67 |
| Graphite | 0.10 | 0.09 | 0.11 |
| Potassium nitrate | 0.78 | 0.70 | 0.82 |
| Calcium carbonate | 0.79 | 0.71 | 0.83 |
| Sodium sulfate | 0.19 | 0.17 | 0.20 |
| Tin dioxide | 1.18 | 1.07 | 1.25 |
| | 100.00 | 100.00 | 100.00 |

Thermochemical properties associated with the compositions given in Table 2 were calculated with the TCC (ThermoChemical Calculations) code [2]. The results of thermochemical calculations for the charge density 0.2 g/cm$^3$ are given in Table 3.

**Table 3. WC 870 (lot A.L. 45137) thermochemical characteristics (TCC code, $\Delta$ = 0.2 g/cm$^3$)**

| Characteristic | Overall composition | Deterred layer | Undeterred layer |
|---|---|---|---|
| Flame temperature [K] | $T_c$; 2750 | $T_{1,c}$; 1978 | $T_{2,c}$; 3189 |
| Covolume [m$^3$/kg] | $\alpha$; $0.930 \cdot 10^{-3}$ | $\alpha_1$; $0.981 \cdot 10^{-3}$ | $\alpha_2$; $0.907 \cdot 10^{-3}$ |
| Specific heats ratio | $\kappa$; 1.241 | $\kappa_1$; 1.266 | $\kappa_2$; 1.227 |
| Molar mass [g/mol] | $\mu$; 23.947 | $\mu_1$; 21.204 | $\mu_2$; 25.865 |
| Propellant force* [J/kg] | $f$; 954800 | $f_1$; 775600 | $f_2$; 1025100 |

* $f = \frac{\mathcal{R}}{\mu} \cdot T_c$; $\mathcal{R}$ – universal gas constant (8.3144 J mol$^{-1}$ K$^{-1}$)

The linear burning rate of propellants as a function of pressure is commonly described for interior ballistic calculations by an equation of the form $r = ap^n + b$. Experience has indicated that the linear burning rate of propellant increases with the flame temperature. This observation led to suggestions for empirical correlations between the flame temperature of propellant compositions and their burning law coefficients (a, b and n) in the equation $r = ap^n + b$.

From the calculated flame temperatures of deterred-contained and undeterred layer of propellant grain (Table 3) the burning rate coefficients of these layers can be determined by the use of empirical correlations. Three correlations were used in this study as follows ($r$ [mm/s]; $p$ [MPa]):

- Muraour [3]:

$$r = 0.078 \cdot e^{0.709(T_c/1000)} p + 0.5 , \qquad (5)$$

- Goldstein [4]:

$$r = 827.76 \cdot e^{-8.15+8.62\cdot 10^{-4} T_c} p^{0.7} , \qquad (6)$$

- Riefler i Lowery [5]:

$$r = \left(8.3956 \cdot 10^{-4} T_c - 0.834\right) p^{0.8053} . \qquad (7)$$

A survey of calculated coefficients a, b and n in the $r = ap^n + b$ burning law for overall composition, deterred and undeterred layer of WC 870 (lot A.L. 45137) propellant is given in Table 4.

**Table 4. Parameters a, b and n in WC 870 (lot A.L. 45137) propellant burning law $r = ap^n + b$ ($p$ [bar], $r$ [m/s])**

| | | $a \cdot 10^4$ | $b \cdot 10^4$ | n |
|---|---|---|---|---|
| Miraour | Overall composition | 0.548 | 5.0 | 1.0 |
| | Deterred layer | 0.317 | 5.0 | 1.0 |
| | Undeterred layer | 0.748 | 5.0 | 1.0 |
| Goldstein | Overall composition | 5.104 | 0 | 0.7 |
| | Deterred layer | 2.624 | 0 | 0.7 |
| | Undeterred layer | 7.452 | 0 | 0.7 |
| Riefler & Lowery | Overall composition | 2.309 | 0 | 0.8053 |
| | Deterred layer | 1.294 | 0 | 0.8053 |
| | Undeterred layer | 2.886 | 0 | 0.8053 |

## 3. INTERIOR BALLISTIC MODEL

The linear burning rate of propellant is usually expressed as a change in time of a burned distance of propellant grain ($r = \mathrm{d}e/\mathrm{d}t$). Thus, the following expression holds during combustion of deterred layer of propellant grain:

$$\frac{\mathrm{d}\left(e/e_0\right)}{\mathrm{d}t} = \frac{1}{e_0}\left(a_1 \cdot p^{n_1} + b_1\right) \qquad (8)$$

where: $e_0$ is half of the initial web of propellant grain, $e$ is burned distance of propellant grain, $p$ is mean (ballistic) pressure of propellant gas, $t$ is time and $a_1$, $b_1$ and $n_1$ are coefficents in deterred layer burning law (Table 4).

The mass fraction of burned propellant is defined by the propellant grain form function:

$$z = ff_1\left(\frac{e}{e_0}\right) + ff_2\left(\frac{e}{e_0}\right)^2 + ff_3\left(\frac{e}{e_0}\right)^3 \qquad (9)$$

where $ff_1$, $ff_2$ i $ff_3$ are the form function coefficients.

The mass fraction of burned propellant at the end of the deterred layer combustion ($z_D$) is obtained from (9) for the burned distance of propellant grain equal to the deterrent penetraion depth ($e = e_D$).

The combustion process of deterred propellant can be divided in two phases.

In the first phase only the deterred layer combustion takes place. This phase lasts as long as $e \le e_D$, that is $\boxed{0 < z < z_D}$.

The Noble-Abel equation of state for propellant gases originated from the deterred layer combustion is:

$$p = \frac{\omega z \dfrac{\mathfrak{R}}{\mu_1} T}{W_0 + sX - \dfrac{\omega}{\rho}(1-z) - \omega z \alpha_1} \qquad (10)$$

where: $T$ is mean temperature of propellant gas, $\omega$ is propellant charge mass, $W_0$ is propellant chamber volume, $s$ is gun tube cross-sectional area, $X$ is projectile displacement, $\rho$ is propellant density, $\mu_1$ is molar mass of propellant gas from deterred layer combustion and $\alpha_1$ is covolume of propellant gas from deterred layer combustion.

The energy equation in this phase of propellant combustion is:

$$\frac{\omega z\left(f_1 - \dfrac{\mathfrak{R}}{\mu_1} T\right)}{(\kappa_1 - 1)} = \frac{1}{2}\varphi m_{pr} V^2 \qquad (11)$$

where: $f_1$ is force of propellant deterred layer, $\kappa_1$ is specific heats ratio of gas ($c_p/c_v$) from deterred layer combustion, $m_{pr}$ is projectile mass, $\varphi$ is coefficient of projectile fictitious mass and $V$ is projectile velocity.

Combining (10) and (11) the following expression is obtained for mean (ballistic) gas pressure:

$$\boxed{p = \frac{\omega z f_1 - \dfrac{\kappa_1 - 1}{2}\varphi m_{pr} V^2}{W_0 + sX - \dfrac{\omega}{\rho}(1-z) - \omega z \alpha_1}} . \qquad (12)$$

In the developed interior ballistic model the equation (12) is used for gas pressure calculation at each integration step of differential equations.

Equation (12) is identical in form with equation used in lumped parameters interior ballistic models for propellant charges composed of undeterred propellants.

The second phase of propellant combustion starts at the moment when combustion of deterred layer is terminated ($e = e_D$; $z = z_D$). In this phase only the combustion of undeterred layer occurs, creating behind a projectile the mixture of deterred and undeterred layer combustion products. The composition of this mixture is different at each moment. Mass fraction of burned propellant is $\boxed{z_D < z < 1}$.

Equation of state of mixture is:

$$p = \frac{\omega z_D \dfrac{\mathfrak{R}}{\mu_1} T + \omega(z - z_D)\dfrac{\mathfrak{R}}{\mu_2} T}{W_0 + sX - \dfrac{\omega}{\rho}(1-z) - \omega z_D \alpha_1 - \omega(z - z_D)\alpha_2} . \qquad (13)$$

Energy equation is:

$$\frac{\omega z_D\left(f_1-\frac{\mathfrak{R}}{\mu_1}T\right)}{(\kappa_1-1)}+$$
$$+\frac{\omega(z-z_D)\left(f_2-\frac{\mathfrak{R}}{\mu_2}T\right)}{(\kappa_2-1)}=\frac{1}{2}\varphi m_{pr}V^2. \quad (14)$$

In order to combine (13) and (14) by elimination of temperature $T$, the principle of mixture of deterred and undeterred propellant layer combustion products is introduced. At each moment of the combustion process the propellant force of instantaneous mixture ($f^*$) is given by the following relation:

$$\omega z f^* = \omega z_D f_1 + \omega(z-z_D) f_2. \quad (15)$$

Propellant force, covolume and specific heats ratio of gaseous mixture are defined by expressions:

$$f^* = \frac{z_D}{z} f_1 + \left(1-\frac{z_D}{z}\right) f_2$$
$$\alpha^* = \frac{z_D}{z} \alpha_1 + \left(1-\frac{z_D}{z}\right) \alpha_2$$
$$\kappa^* = \frac{z_D}{z} \kappa_1 + \left(1-\frac{z_D}{z}\right) \kappa_2. \quad (16)$$

The mean pressure of propellant gas mixture is now given by equation equivalent to (12), but with instantaneous mixture characteristics $f^*$, $\alpha^*$ and $\kappa^*$. Finally, the gas pressure is defined by the following expression:

$$p = \frac{\omega z_D f_1 + \omega(z-z_D) f_2 - \frac{\kappa^*-1}{2}\varphi m_{pr}V^2}{W_0 + sX - \frac{\omega}{\rho}(1-z) - \omega z \alpha_1 - \omega(z-z_D)\alpha_2}. \quad (17)$$

Equation (17) is also valuable after completion of propellant combustion, with z = 1 and with constant value of $\kappa^*$ obtained from (16) for z = 1.

The PERFFL code for the computation of whole interior-ballistic cycle of ammunition whose propellant charge is composed of deterred propellant is created.

The model verification is carried out by comparison with American experimental results of 20 mm M55A2 ammunition firings from 20 mm D20 gun [6]. The propellant charge of this ammunition consists of WC 870 ball propellant.

In existing lumped parameters interior ballistic model (GRAD code) and in PERFFL code the grain geometry of a given ball propellant is expressed as the equivalent mean diameter $d_{eq}^{(S)}$ based on particle surface area. The equivalent mean diameter is calculated from the following equation with the particle size distribution obtained from a sieve analysis of the propellant.

$$d_{eq}^{(S)} = \sqrt{\phi_1 d_1^2 + \sum_2^{n-1} \phi_i d_{m,i}^2 + \phi_n d_n^2}. \quad (18)$$

The SFERFL computer code is created in order to achieve more adequate treatment of ball propellant combustion. In this code the combustion of each granulation is considered separately in such a way that $i$-th granulation is represented as a ball propellant with mean grain diameter $d_{m,i}$.

In Table 5 the comparison of computational results of the main interior ballistic parameters (projectile muzzle velocity – $V_0$, maximum ballistic pressure – $p_m$) with experimental data is given. The WC 870 ball propellant characteristics (force, covolume, specific heats ratio, burning law) given in Tables 3 and 4 were used for interior ballistic calculations (burning law coefficients according to Miraour).

**Table 5. Comparison of computational results for main IB parameters with experimental data**

| | $V_0$ [m/s] | $p_m$ [bar] |
|---|---|---|
| Experiment | 1045 | 2950 |
| GRAD code | 1051 | 5694 |
| PERFFL code | 1047 | 3228 |
| SFERFL code | 1036 | 3080 |

From Table 5 it is clear that GRAD code treat inadequately the deterred propellant combustion. It was not possible to obtain computational results close enough to the experimental data by the input parameters variations within the wide limits of physically realistic values.

Computational results similar to corresponding experimental data were obtained with PERFFL and SFERFL codes at the very start. The similarity of results was easily attained in both cases by the convenient adjustment of input parameters ("lumped parameters" models).

It seems that SFERFL code has not an appreciable advantage over PERFFL code in estimations of main interior ballistic parameters. This indicates that the treatment of ball propellant combustion by the equivalent mean diameter based on particle surface area is quite satisfactory in most cases.

The SFERFL code is expected to show significant advantages during considerations of such practical interior ballistic problems where the whole curve of pressure changes in time is important.

## 4. CONCLUSIONS

Based on previous considerations, the following conclusions can be drawn:

- The deterred layer characteristics of propellant grain must be taken into consideration in interior ballistic calculations for successful design of high performance propelling charges. Existing interior ballistic models are incapable to treat adequately the combustion of deterred propellants;
- The new model is developed for interior ballistic cycle calculations of systems with propelling charge composed of deterred propellants. The special version of computer code is also created for calculations of ball propellants combustion;
- The procedure is defined for determination of deterred propellants characteristics, which are

necessary for interior ballistic cycle calculations;
- The verification of developed models is carried out through the comparison with American experimental data of 20 mm ammunition with propellant charge composed of deterred ball propellant.

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## ТРЕТИРАЊЕ ФЛЕГМАТИЗОВАНИХ БАРУТА У УНУТРАШЊЕБАЛИСТИЧКИМ ПРОПАЧУНИМА


**Дејан Мицковић**



У раду је дат поступак одређивања карактеристика флегматизованог барута које су неопходне као улазни параметри за унутрашњебалистичке прорачуне. Приказане су основне специфичности развијеног модела за прорачун унутрашњебалистичког циклуса система са барутним пуњењем од флегматизованог барута. Верификација модела извршена је упоређењем прорачунских резултата са америчким експерименталним резултатима опаљења муниције калибра 20 mm са барутним пуњењем од сферичног барута.