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Modelling of Heat Loss in Closed Vessels during Propellant Burning

U.P. Kulkarni

High Energy Materials Research Laboratory, Pune - 4 021

and

Smita D. Naik

Institute of Armament Technology, Pune – 4 025

ABSTRACT

Closed vessel techniquel is essentially used to determine the force constant, vivacity and the burning rate of gun propellants. In fact, it is the only method to find out these three parameters experimentally. It is a well-known fact that however small the propellant burning time may be, there will be heat loss to the walls of the vessel due to conduction, convection, radiation and also due to the expansion of the vessel. This fact necessitates applying correction to the observed maximum pressure in the experiment. An analysis is presented in this paper as to how this heat loss can be modelled along with discussion about other models reported in this field.

NOMENCLATURE

- F Force constant of the propellant
- C Charge weight of the propellant
- K_0 Chamber volume
- ρ_p Loading density of the propellant
- b Co-volume of the propellant gases
- D Web size of the propellant grain
- z Fraction of charge burnt at any instant t

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- f Fraction of web remaining at any instant t
- P Pressure at any instant t
- V Specific volume

- β Burning rate coefficient
- *n* Burning rate index
 - Specific heat of gas at constant volume
- T Temperature of the gas complex
- T_e Flame temperature
- S Surface area of the inner walls of the vessel
- θ Form factor of the propellant
- P_m Observed maximum pressure within the vessel
- ρ Density of the gas complex
- v Mean velocity of the gas molecules

1. INTRODUCTION

The burning of the propellant in the closed vessel (CV) follows Piobert's law and hence can be given by the following form function:

$$z = (1-f)(1+\theta f) \tag{1}$$

and the index law of burning is

$$-D\frac{df}{dt} = \beta P^n \tag{2}$$

The force constant (F) is computed from a CV experiment by recording the maximum pressure (P_m) developed within the chamber when an accurately known quantity of the propellant is burnt under constant volume conditions and applying Nobel and Abel's equation of state¹, viz.,

$$P_m(V-b) = F \tag{3}$$

While using the above equation, an assumption is made that the temperature of the propellant gases (T) is equal to the adiabatic flame temperature (T_e) of the propellant during the entire period of burning. In reality, the actual equation is:

$$P(V-b) = F \frac{T}{T_e}$$
(4)

Due to the ensuing heat loss during the burning period, T never reaches the adiabatic T_e but comes quite close to it. An estimate made is that the temperature varies from 0.97 $T_e' - 0.99 T_e$ in the region z = 0.1-1.0. In the semi-empirical approach towards modelling of heat loss in the subsequent analysis, the discussion of energy loss due to various factors is based on this assumption. In the theoretical approach using experimental data, a linearised solution is obtained which accounts for the variation of T as a function of web remaining (f).

2. EMPIRICAL METHODS

The literature survey reveals that the first quantitative corrections to be applied to P_m for various types of propellants² are given in Table 1.

Propellant type	Percențage correction
N or NFQ	3:7 + 15D
NQ or NQF	12.5 + 15D
WM or SC	0,9 + 15D
HW or HSC	0.9 + 15D

In the above listing, the prefix H stands for the hotter variety of the propellant. WM, SC and HSC are different types of cordite. It is evident from the above that the cooler propellants (with adiabatic T_e less than about 3000 K) require a larger correction factor, while the hotter wariety requires a smaller one. These corrections are normally applied in CV experiments with a chamber volume (K_0) of 700 ml and a propellant loading density (ρ_p) of 0.2 g/cc. The chamber pressures are of the order of 250 MPa-300 MPa.

The mean temperature (T) of the gases at any time (t) as suggested by Crow and Grimshaw³ can be obtained from:

$$CC_{v} z(T_{e} - T) = cP^{2}S + (T - T_{i})aS\sqrt{t}$$
 (5)

The above formula equates the loss of heat up to t to the energy (in heat units) lost in expanding the vessel and the heat lost to the vessel. T_i indicates the initial temperature of the internal surface of the vessel, a and c being the constants of the vessel. However, it is unclear as to which value of T_i needs to be taken for computations. Moreover, this parameter is difficult to measure.

Vittal⁴ has discussed an empirical model to obtain correction for the heat loss by carrying out firings in CV at different loading densities. This is done to evaluate the constants appearing in the heat loss function. The computation involves the knowledge of thermochemical data related to the propellant under test and also the temperature of the inner walls of the vessel which is a difficult quantity to measure. However, a simplistic empirical model is discussed here. As discussed in Vittal's model, when the propellant is burnt in CV, the rate of fall of pressure is proportional to the pressure immediately after reaching P_m . The type of CV, the propellant and the ρ_p defines this relationship. This fact can be used to determine the corrections to be applied to the observed P_m . The advantage of this method is that it can be applied effectively even when the thermochemical data of the propellant is not known.

To start with, the p-t data is obtained at a sufficient number of points during the duration of say, 20 ms after P_m . This then is converted to rate of change of pressure dp/dt versus P data. Using commercially available software like GRAPHER, a best fit is obtained for dp/dt in terms of P. For a number of firings with same conditions, one gets the equation:

$$\left.\frac{dp}{dt}\right|_{k} = K_{i}P + A \tag{6}$$

where $(dp/dt)_c$ stands for the rate of fall of pressure in the cooling portion immediately after P_m . Using this data, the average values of K_i 's and A_i 's are obtained. Equation (6) can be rewritten as

$$\left(\frac{dp}{dt}\right)_{c} = KP_{1} + A$$
(7)

where K is the average of K_i 's and A is the average of A_i 's. The actual rate of fall of pressure is given by

$$\frac{dp}{dt} = \left(\frac{dp}{dt}\right)_{r} + \left(\frac{dp}{dt}\right)$$
$$= \left(\frac{dp}{dt}\right)_{r} + KP_{r} + A$$
(8)

where the subscript r stands for recorded.

By integrating Eqn (8), the corrected pressure is obtained as

$$P = P_r + K \int P_r dt + A \int dt$$
(9)

where P on the right has been replaced by P_r . The error introduced due to this is negligible.

¹ For the corrected maximum pressure (P_{mc}) , one can write:

$$P_{mc} \quad P_{mr} + K \int P_{mr} dt + A \int dt$$
$$= P_{\star} + K P_{mr} t + At$$

where P_{mr} is the recorded maximum pressure and t is known from the experimental data. In this way, one can find out the corrections for different CV for various propellants and loading densities.

3. DISTRIBUTION OF ENERGY LOSS – SEMI-EMPIRICAL MODEL

During the major part of burning of the propellant in CV, variation in T of the gas complex is assumed to vary between 0.97 $T_e - 0.99 T_e$ in the region z = 0.1-1.0. It is also assumed that this variation is linear. With this, the following points emerge:

(a) Had there been no heat loss, the gases would have been at the adiabatic T_e . Hence, at any instant the heat lost is given by

$$H_L = C_z C_v (T_e - T) \tag{1}$$

For the propellant NQ/M 028 (reported T_e 2850 K), T is given as a function of z by a linear relation:

$$T = 2758.167 + 63.333z$$

where

 $T = 0.97 T_e$ at z = 0, and $T = 0.99 T_e$ at z =

(b) Over the burning period, the following energy losses will occur:

• Energy is lost in expanding the vessel and also in compressing the ablative material used in the closing plugs. It is estimated¹ that this energy loss is maximal of the order of 1 per cent of the total energy. This is termed as the strain energy and is theoretically proportional to P^2 and also to S.

• The convective heat loss can be allowed for in a simple manner. The kinetic energy of the gas molecules is given by $\frac{1}{2} \rho v^2$ which is lost to the walls of the vessel during simple convection. By the kinetic theory of gases, the velocity of the gas molecules is given by $\sqrt{2P/\rho}$. Hence, the energy lost due to convection becomes proportional to the pressure.

$$\frac{1}{2}\rho\left(\sqrt{\frac{2P}{\rho}}\right)^2 = P$$

• Another major source of energy loss is due to radiation and transient conduction. This can be assumed proportional to the time of burning as well as the mass rate of burning, hence is proportional to the product t.dm/dt.

Then the energy balance equation becomes:

$$CzC_{\nu}(T_{e}-T) = c_{1}P^{2}S + \alpha P + kt\frac{dm}{dt}$$
(13)

where c_1 , α and k are the constants to be determined. These have the following dimensions:

 $c_1 \rightarrow M^{-1} L^2 T^2$ $\alpha \rightarrow L^3$ $k \rightarrow L^2 T^{-2}$

Using experimental data, it was observed that when the heat loss was summed over the burning period from z = 0:1-1.0 and was compared with the total energy (assuming adiabatic T_e throughout the above burning period), the energy loss was about 6 per cent of the total energy. It may be recalled that during the CV experiments, the energy loss is assumed⁴ to be 4-10 per cent.

Let

$$E = c_1 P^2 S + \alpha P + kt \frac{dm}{dt} - C z C_v (T_e - T)$$
(14)

Then, one ideally expects that E = 0. Efforts were made to obtain the values of the three constants using least square method while the values of P^2 , P, z ($T_e - T$), t.dm/dt were substituted summed over the burning period from 10–100 per cent from several CV experiments. However, the method failed to obtain consistent solutions at minimum error (all the three constants need to be positive valued).

The above problem can be analytically solved by plotting a surface in the (c_1, α, k) space. These are illustrated for a 100 ml and a 700 ml vessel in Fig. 1. These clearly show a latger percentage of heat loss for the 100 ml vessel whose S/V ratio (surface area per unit volume) is higher than that for the 700 ml vessel.

Also (α, k) relations for different values of c_1 are given for both the vessels in Figs 2 and 3. With this semi-empirical approach, the following observations are made:

For a given value of c_1 , α and k vary linearly along a straight line.

For a given value of α , k and c_1 vary linearly along a straight line!

• Similarly, for a given value of k, α and c_1 vary linearly along a straight line.

As c_1 increases, k decreases, α increases.





Figure 1. Surfaces in the space (c_1, α, k)



Figure 2. (α, k) variation for different values of c_1 for 100 ml vessel.

However, for each point individually, one cannot conclude that the error is minimum. For a given propellant and for the selected value of c_1 based on z, it is left to the user to obtain the most likely values of α and k from the solution set.

4. OTHER MODELS

In general, it has been observed that there is always a difference between the theoretically calculated and the experimentally observed values of pressure in CV due to heat loss to the walls of the vessel. These heat loss can be modelled with the help of different parameters like co-volume, pressure drop, change in pressure, etc.

The equation of state considered for the theoretical model is that of Noble and Abel¹ as the pressure range involved is normally < 500 MPa. However, while dealing with very high chamber pressures (above 700 MPa or loading densities of 0.4 g/cc and above), this ideal equation of state can be modified to a truncated virial equation as discussed by Wang and Qu⁵. They suggest the use of truncated virial equation given by

$$\frac{P}{n\rho_g R_u T} = +B(T)n\rho_g + C(T)(n\rho_g)^2$$
(15)

where ρ_g is the gas molar density and R_u is the universal gas constant, B(T) and C(T) are the second and third virial coefficients.

For very small volume CVs, the co-volume of the propellant gases becomes an important parameter and the determination of heat loss and consequent pressure loss has been discussed by Hendricks and Both⁶. In this work, heat loss has been taken in terms of pressure drop as well as co-volume. The experimental value of co-volume can be expressed as a function of the thermodynamically calculated value as

$$\eta^* = \frac{\eta_0}{1 - A} \qquad \frac{B}{-A} \tag{16}$$

with

$$A = \frac{p_1}{p_{\max_1}} - \frac{p_2}{p_{\max_2}}, \quad B = \frac{\Delta_2 p_1 - \Delta_1 p_2}{\Delta_1 \Delta_2 (p_{\max_1} - p_{\max_2})}$$

 p_{\max} is the maximum pressure and p is the pressure drop. The suffices 1 and 2 are for the loading densities Δ_1 and Δ_2 , respectively. The pressure loss can be found by the formula:

$$p_{D} = \frac{F_{0}}{\eta_{0}} - p_{\max_{\alpha}} - p_{\max_{\alpha}}$$
(17)

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where F_0 and $p_{\max_{ex}}$ are the calculated force constant, and the experimental maximum pressure, and p_D is the loss of pressure.

For a 25 ml CV and a single-base propellant, the estimated pressure loss (in MPa) is given by

$$p_{D} = 11.6 + 0.059 * P_{\text{max}} \tag{18}$$

Parametric study of heat loss in a CV has been carried out by Mailette⁷, *et al.* It is assumed that the amount of heat loss to the walls of the vessel Q_w between propellant ignition and burnout can be evaluated. With this, the amount of heat lost during time Δt can be modelled in two ways.

In the first approach, the heat transfer is assumed to be constant throughout the combustion process. ΔQ_w , the amount of heat lost during time Δt , is calculated as¹

$$\Delta Q_{w} = Q_{w} \frac{\Delta t}{t - \tau t_{ign}}$$
⁽¹⁹⁾

where $t_{p_{\text{max}}}$ and t_{ign} are the time to reach maximum pressure and time for ignition, respectively.

The second approach assumes that the heat transfer is linearly dependent on the pressure measured during the experiment. Hence,

$$\Delta Q_{w} = Q_{w} \frac{\Delta P}{P_{obs}^{max} - P_{ign}}$$
(20)

where P_{obs}^{max} is the maximum pressure in the experiment and ΔP is the pressure difference in the desired time interval. Using the above approaches, a variation up to 8.5 per cent has been found in the burning rates of multitubular propellants at the same pressure and so there is a need for an improved heat loss model.

5. THEORETICAL MODEL

Based on the knowledge of burning behaviour of the propellant in a CV, a theoretical model can be attempted which takes into account the varying temperature of the gas complex. Here, T/T_e is considered as a linear function of f or z.





Then the equation of state can be written as

$$P(V-b) = F(a_0 f + b_0)$$
(21)

where a_0 and b_0 are the constants to be determined.

Substituting for $(V-b)_{p}$

$$P\left(\frac{\delta}{z} + \Delta\right) = F(a_0 f + b_0)$$
(22)

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where
$$\delta = \frac{K_0 - \frac{C}{\rho_p}}{C}$$
 and $\Delta = -b + \frac{1}{\rho_p}$
Substituting $z = (1 - f)(1 + \theta f)$ in Eqn (22)
 $P\{\delta + \Delta(1 + (\theta - 1)f - \theta f^2)\} = F(\alpha I_0 f^{3^1} + \alpha_1 f^2 + \alpha_2 f + \alpha_3)$
(23)

where

$$\alpha_0 = -a_0\theta, \ \alpha_1 = a_0(\theta - 1) - b_0\theta$$

$$\alpha_2 = b_0(\theta - 1) + a_0, \ \alpha_3 = b_0$$

Differentiating Eqn (23) and also using the relation [Eqn (2)], one gets:

$$D\left(\frac{dp}{dt}\right)\left\{\delta + \Delta(1 + [\theta - 1]f - \theta f^{2})\right\} + (\Delta\beta P^{n+1})^{*}$$

$$(1 - \theta + 2\theta f) + F\beta P^{n}(3\alpha_{0}f^{2} + 2\alpha_{1}f + \alpha_{2}) = 0$$

Eliminating f between Eqns (23) and (24)

$$\begin{cases} D \frac{dp}{dt} (\delta + \Delta) + \Delta \beta (1 - \theta) P^{n+1} + F \beta \alpha_2 P^n \\ + \begin{cases} -\sigma r & dt \\ -\theta & D\Delta \frac{dp}{dt} + 3F \beta \alpha_0 P^n \end{cases} N^2 = 0 \end{cases}$$
(25)

where

$$N = D^{2} \left(\frac{d\mu}{dt}\right)^{2} \left(-Fb_{0}\Delta\delta \theta^{2}\right) - P^{n+2} \left(\frac{dp}{dt}\right)$$

$$\begin{bmatrix} D\Delta^{3} \beta\theta^{2} (\theta-1) \end{bmatrix} - P^{n+1} \left(\frac{dp}{dt}\right)$$

$$\begin{bmatrix} a_{0} F\beta\Delta\theta^{2} D(11\delta+12\Delta) + 2Fb_{0}\Delta^{2} D\beta\theta^{2} (\theta-1) \end{bmatrix}$$

$$+ P^{n} \left(\frac{dp}{dt}\right) \begin{bmatrix} a_{0}^{2} F^{2} D\beta(\delta+\Delta)\theta (\theta-1) + a_{0}b_{0}\theta^{2} \end{bmatrix}$$

$$F^{2} D\beta(4\Delta-\delta) - F^{2}\theta^{2} (\theta-1)\Delta\beta b_{0}^{2} \end{bmatrix}$$

$$+ P^{2n+2} \begin{bmatrix} a_{0}\theta^{2} (\theta-1)F\Delta^{2}\beta^{2} \end{bmatrix}$$

$$-P^{2n+1}[a_0^2 F^2 \beta^2 \{\Delta \theta (\theta - 1)^2 + \theta^2 (9\delta + 8\Delta)\} -4a_0b_0F^2 \beta^2 \Delta \theta^2 (\theta - 1)] +P^{2n}[a_0^3 F^3 \beta \theta (\theta - 1) + a_0^2 b_0 F^3 \beta^2 \theta (\theta^2 + 6\theta + 1) - a_0b_0^2F^3 \beta^2 \theta^2 (\theta - 1)]$$

and

$$D_{ij} = D^{2} \left(\frac{dp}{dt}\right)^{2} \left[Fa_{0}\theta(\delta + \Delta)\Delta - Fa_{0}\Delta^{2}\theta^{2}\right]$$

$$+ P_{i}^{n+2} \left(\frac{dp}{dt}\right) \left[-2\theta^{3}\Delta^{3}D\beta\right] + P^{n+1} \left(\frac{dp}{dt}\right)$$

$$\left[2Fa_{0}^{1}\theta^{2}\Delta^{2}D(\theta - 1)\beta + 4F\theta^{3}\Delta^{2}D\beta b_{0}\right]$$

$$+ P^{n} \left(\frac{dp}{dt}\right) \left[-a_{0}^{2}F^{2}\theta(\theta - 1)^{2}\Delta D\beta - 2a_{0}b_{0}\theta^{2}\right]$$

$$\left(\theta - 1)F^{2}D\beta\Delta + a_{0}^{2}\theta^{2}F^{2}D\beta(3\delta - 2\Delta)\right)$$

$$-2b_{0}^{2}\Delta\theta^{3}DF\beta$$

$$- 2a_{0}\theta^{3}\Delta^{2}\beta^{2}P^{2n+2} + P^{2n+1}\left[2a_{0}^{2}\theta^{2}(\theta - 1)\right]$$

$$F^{2}\beta^{2}\Delta + 4a_{0}b_{0}\theta^{3}F^{2}\beta^{2}\Delta\right]$$

$$+ P^{2n}\left[-2a_{0}^{3}\theta(\theta - 1)^{2}F^{3}\beta^{2} - 2a_{0}^{2}b_{0}\theta^{2}(\theta - 1)\right]$$

$$F^{3}\beta^{2} - 2a_{0}b_{0}^{2}\theta^{3}F^{3}\beta^{2} - 6a_{0}^{3}\theta^{2}F^{3}\beta^{2}\right]$$

Treating Eqn (25) as an error expression, the values of a_0 , b_0 , n and β are obtained by least square method. $P^m (dp / dt)^n + type$ of products, P^x , $(dp / dt)^y$ type of values are obtained from the CV experimental data, summed over the entire burning period.

However, the expressions involved are nonlinear and complicated. These cannot be solved easily to get consistent solutions. An approximate solution can be obtained by using linear burning law and solving the linearised simultaneous equations in a_0 and b_0 .

6. ILLUSTRATION

6.1 Propellant

NQ/M028 with loading density 0.2g/cc in 700 ml CV.

6.2 Values

 $F = 1037.2 \,\text{J} / \text{g}, n = 1, \beta = 0.1409$

 $\theta = -0.172, \rho_p = 1.668 \text{ g/cm}$

Linearised equations in a_0 and b_0 after substituting the above values are:

1466.500996 a_0 + 35.347579 b_0 = 4.6122783 3362.502299 a_0 + 75.906514 b_0 = 5.4664687 These yield solutions: a_0 = -0.021 b_0 = 0.994

This emphasises the fact that during the burning period, T/T_e varied from 0.973 at f close to 1 (z close to zero) to 0.994 when f is close to zero (z close to 1); that is a variation in the gas temperature from 0.973 $T_e - 0.994 T_e$. This closely agrees with the assumptions made while constructing the semi-empirical model. The temperature variation profile as a function of z is shown in Fig. 4.



Figure 4. Temperature profile in closed vessel firing

7. DISCUSSION & CONCLUSIONS

The temperature variation of the gas complex during the early stages of burning of the propellant in the CV is not well understood. Empirical, semi-empirical and theoretical models have been discussed to analyse the problem of heat loss and also the necessary corrections needed to be applied to the observed maximum pressure in the experiment. Semi-empirical model helps analytically-to understand the distribution of energy losses in a CV experiment due to various factors. Study of the theoretical model with the help of experimental data and finding the approximate solutions to the linearised equations in a_0 and b_0 provides a reasonably good insight into the temperature variation of the gas complex throughout the burning period as described in the illustration. The future scope of the work involves finding the optimum parameters for a particular propellant-CV configuration by solving the nonlinear equations discussed in the theoretical model. This will help in better understanding of the phenomenon of propellant burning in CV and may also improve prediction accuracy of energy losses.

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Contributors



Mr UP Kulkarni joined DRDO at the High Energy Material's Research Laboratory (HEMRL), Pune in 1978. He obtained his MSc (Physics) from Karnatak University, in 1977 and MTech (Modelling and Simulation) from IAT, Pune, in 1996. His areas of interest are modelling of rocket and gun propellants.



Dr (Mrs) Smita D Naik obtained her PhD from the University of Poona, Pune, in 1988. She joined DRDO at the Institute of Armament Technology, Pune, in 1987. Her areas of research are flight dynamics and stability analysis. She has published eight papers in national/international journals.