Optimal Calculation of Solid Propellant Burning Equilibrium Ingredients Based on Genetic Algorithm

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Abstract. To aim at defects caused by using Lagrange multiplier to solve equilibrium ingredients in engineering, genetic algorithm based on reduction of dimensionality and mixture rank are adopted in this paper. In genetic algorithm, design dimension is decreased through independence analysis of design variables, and individuals are ranked with violation degree and violation times simultaneously. The method in this paper can solve the problems brought by Lagrange multiplier method, which were unable to effectively deal with quantity equal constraints in equilibrium ingredients optimization and increased the number of unknown variables and calculation difficulties for complex propellant. Moreover, the method can also avoid the problem of computing termination on account of minus value during ingredients calculation, and can be easier to get global optimal solution. Furthermore, an integrated calculation frame of equilibrium ingredients is established by combining equilibrium ingredients optimization model with burning temperature model. Finally, an example is used to verify the method’s validity and feasibility.

1. Introduction

Three classical methods of gradual approximation, minimum G-free energy and Brinkley were usually used to calculate solid propellant burning equilibrium ingredients [1-3]. Although gradual approximation method is simplest, it is unable to compile general procedures for all problems and not suitable for calculation with abundant equilibrium ingredients, so the method is rarely used. In Brinkley method, equations to be solved are linear and the number of equations is fewest, but there are too many coefficient matrixes to input, it is easily to make mistakes. Minimum G-free energy is easily understood and has specific physical significance. Therefore, we mainly discuss minimum G-free energy method in this paper. Formerly, Lagrange multiplier was usually applied to get minimum G-free energy. It can bring about two main problems. Firstly, once the ingredients’ values during the process of optimization were less than zero, optimization calculation would be terminated. Secondly, if equilibrium ingredients were abundant, calculate derivatives is consuming. To avoid above problems, we use a genetic algorithm based on reduction of dimensionality and mixture rank which can deal with equation constraints in optimization to solve G-free energy optimization.
2. Optimization model to calculate equilibrium ingredients

2.1. Objective Function

Here, we can easily select G-free energy as objective function. G-free energy and objective function can be expressed as follows.

\[
\min \Phi = \sum_{i=1}^{L} \left(Y_i^c n_i\right) + \sum_{i=L+1}^{N} \left(-Y_i + \ln n_i + \ln p_e - \ln n_g\right) n_i
\]

(1)

Where \(\Phi = G/RT\), \(G, R, T\) are G-free energy, gas constant and absolute temperature respectively. \(L\) is the number of agglomerate burning ingredients. \(N\) is the number of burning ingredients. \(n_i\) is molar number of the \(i\)-th burning ingredient. \(p_e\) is burning pressure; it is known when calculating equilibrium ingredient. \(n_g\) is total molar number of gas burning ingredients. \(Y_i^c = -G^\theta_{T_i c}/RT\), \(G^\theta_{T_i c}\) is standard molar G-free energy of agglomerate, which can be calculated [4].

\(Y_i = -G^\theta_i/RT\), \(G^\theta_i\) is standard molar G-free energy of gas, which can be calculated [4].

In formula (1), \(n_i\) is variable. When \(\Phi = G/RT\) gets minimum evaluation, corresponding \(n_i\) is molar number of the \(i\)-th equilibrium ingredient, that's what we asked for.

2.2. Constrains

Because preburning mass (i.e. propellant mass) must be equal to afterburning mass, mass conservation equations are constraints of optimization, it can be expressed as follows.

\[
\sum_{i=1}^{N} A_{k i} n_i \geq 0 \quad (k = 1, 2, \cdots, m)
\]

(2)

Where \(N_k\) is molar number of element in assumed chemical formula, which can be derived from recipe of propellant. 
\(m\) is the number of propellant element. 
\(A_{k i}\) is molar number of the \(k\)-th element contained in one mole of the \(i\)-th burning ingredient.

2.3. Solving algorithm

At past, the classic method to solve the model was Lagrange multiplier. As thus, \(n_i\) may be negative during optimization, and optimization could be terminated. Moreover, most of constrains in optimization model are equations, the number of equality constraints equals to the number of propellant element. The propellant recipe is more complex, the constraints’ number is larger. It also probably increases difficulty to solve optimization model. Hu proposed a genetic algorithm to solve optimization problem with equality constrains [5]. In this paper, we will use the genetic algorithm to solve the optimization model of equilibrium ingredients calculation. In the genetic algorithm, there are two keys, which are called reduction of dimensionality and mixture rank.

In the first key point, all variables are divided into independent and dependent variables through independence analysis, dependent variables are functions of independent variables (i.e. design variables) and can be obtained by solving equations transformed from equality constrains. In this way, the number of design variables can be reduced and all new constraints in the optimization model are inequality, so it is called reduction of dimensionality. But it should be noted to avoid ill-condition equations when selecting design variables.
In the second key point, individuals are ranked by referring to the multi-objective idea. That is to say, violation degree and violation times of constrains are simultaneously used to valuate individuals, and violation times of constrains sometimes are more important than violation degree, which is more practical.

Using genetic algorithm based on reduction of dimensionality and mixture rank, which is called RMGA in this paper, we can summarise main steps of calculating equilibrium ingredients as follows.

1) analyze the rank of mass conservation equations to determine independent variables (i.e. design variables) and dependent variables.
2) generate initial population of design variables.
3) calculate values of dependent variables through solving mass conservation equations based on the values of independent variables.
4) calculate minimum G-free energy of population.
5) calculate constrains’ violation times of population.
6) rank population according to minimum G-free energy and violation times of constrains.
7) generate new population by selection, cross, and mutation.
8) calculate new values of dependent variables through solving mass conservation equations based on the new values of independent variables.
9) calculate minimum G-free energy of population.
10) calculate constrains’ violation times of population.
11) combine old and new population, then rank population.
12) select and generate new population. If evolution algebra is less than the given number, then transfer to 7). Otherwise terminate and output results.

Moreover, because \( n_i \) could be zero, \( \ln n_i \) in formula (1) wouldn’t be calculated. This problem can be avoided by the following agreement.

(1) let \( n_i \geq \varepsilon_i \quad i = 1,2,\cdots,N \)

(2) if \( \zeta > n_i \geq \varepsilon_i \), then \( n_i \approx 0 \), so this burning product should be omitted.

Where \( \varepsilon_i \) and \( \zeta \) are also given small decimal fractions.

2.4. Burning temperature calculation[3]

From optimization model, we can see it is necessary to get burning temperature of \( T_c \) when calculating equilibrium ingredients. Unfortunately, burning temperature is also unknown. But when molar number of equilibrium ingredients is known, it can be derived from principle of energy conservation, in other words, solid propellant’s total enthalpy of \( I_p \) and burning products total enthalpy of \( I_m \) are conservative. In this way, we can get burning temperature by solving the following equation, namely

\[
\sum_{i=1}^{m} \left[ H_{f_p}^T + c_i(T_i - T_f) \right] \cdot q_i = \sum_{i=1}^{N} \left( H_{f_p}^T_{298} + \int_{T_f}^{T_i} C_{p_i}dT \right) \cdot n_i \quad (3)
\]

Obviously, the formula (3) is a highly nonlinear equation with respect to \( T_c \). In engineering, linear interpolation method is usually used to solve the formula 3 based on two presupposed temperatures. The method is simple, but two preselected temperatures depending on analyst’s experiences would affect computation accuracy. In this paper, we will use following method. Formula 3 can be transformed as follows.

\[
f(T) = \sum_{i=1}^{m} \left[ H_{f_p}^T + c_i(T_i - T_f) \right] \cdot q_i - \sum_{i=1}^{N} \left( H_{f_p}^T_{298} + \int_{T_f}^{T_i} C_{p_i}dT \right) \cdot n_i = 0 \quad (4)
\]

Here, equation (4) will be solved by secant method [6], so iterative formula is expressed as follows

\[
T_{k+1} = T_k - \frac{f(T_k)(T_k - T_{k-1})}{f(T_k) - f(T_{k-1})} \quad (5)
\]
When $|I_p - I_m| \leq \varepsilon_2$, iteration terminates. Where $\varepsilon_2$ is a given small decimal fraction.

2.5. Calculation steps
According to section 2.1. and section 2.4, we can see burning temperature and equilibrium ingredients are input datum of optimization and burning temperature calculation respectively. So optimization and burning temperature calculation form a nested loop, we can use iteration to solve the problem and get equilibrium ingredients. Hereby, the whole calculation frame (i.e. steps) can be showed by Figure 1.

![Figure 1](image_url)

**Figure 1.** Whole calculation frame

3. Example
Recipe of solid propellant were listed in Table 1, the propellant will be burned at 6.08Mpa, and $T_i$ is 298K, please calculate its equilibrium ingredients.

**Table 1.** Recipe of solid propellant

| Number | Component       | Mass percent | Standard creation enthalpy (KJ/mol) |
|--------|----------------|--------------|------------------------------------|
| 1      | NH₄ClO₄        | 68%          | -291.56                            |
| 2      | Al             | 15.5%        | 0                                  |
| 3      | CaCO₃          | 3.5%         | -1211.66                           |
| 4      | C₂₂₀H₄₄₁O₆₁   | 13%          | -14001.83                          |

Therefore, assumed chemical formula is $Ca_{0.3497}Al_{5.745}C_{7.385}H_{37.262}O_{26.1523}N_{5.7678}Cl_{5.787}$ and $I_p$ is $-6.0935 \times 10^5$cal. There are fifteen kinds of assumed burning products listed in Table 2.

Accordingly, mass conservation equation between preburning and afterburning can be formulated as follows, namely

$$Ax = b$$

Where $x = [x_1, x_2, \cdots, x_{15}]'$
\[
A = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 2 & 2 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
1 & 3 & 1 & 0 & 1 & 0 & 0 & 2 & 0 & 1 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[b = [0.3497 \quad 5.7450 \quad 7.3890 \quad 37.2620 \quad 26.1523 \quad 5.7878 \quad 5.7878]'\]

**Table 2. Assumed burning products**

| code | product | code | product | code | product | code | product |
|------|---------|------|---------|------|---------|------|---------|
| x_1  | CaO(s)  | x_5  | H_2O    | x_9  | H       | x_{13}| NO      |
| x_2  | Al_2O_3(s) | x_6  | N_2     | x_{10}| AlOCl   | x_{14}| CHO     |
| x_3  | CO      | x_7  | HCl     | x_{11}| Cl      | x_{15}| O       |
| x_4  | H_2     | x_8  | CO_2    | x_{12}| HO      |       |         |

Obviously, the rank of first Seventh column of A is full. In this way, the seven burning ingredients, which are CaO(s), Al_2O_3(s), CO, H_2, H_2O, N_2 and HCl, can be regarded as design parameters (i.e. dependent variables), the other eight burning ingredients are design variables. We can get the seven burning ingredients by solving linear equation of mass conservation.

The values of corresponding parameters in calculation are listed as follows.

Initial burning temperatures for iteration are 2000K and 3000K respectively.

Genetic algorithm uses real code, population scale is 20, evolution algebra is 100, cross probability is 0.9, mutation probability is 0.05, simulated binary cross operator and polynomial mutation operator are adopted, cross and mutation distribution index are 20 respectively.

In addition, \( \varepsilon_1 \), \( \varepsilon_2 \) and \( \zeta \) are \( 10^{-5} \), \( 10^{-4} \) and \( 10^4 \) respectively.

Finally, the results of equilibrium ingredients calculation are shown in Table 3.

**Table 3. The results of equilibrium ingredients calculation**

| burning ingredient | the number of moore | burning ingredient | the number of moore |
|--------------------|---------------------|--------------------|---------------------|
| CaO (s)            | 0.3497              | H                  | 0.5485              |
| Al_2O_3(s)         | 2.7391              | AlOCl              | 0.2668              |
| CO                 | 6.4221              | Cl                 | 0.2734              |
| H_2                | 6.9698              | HO                 | 0.3414              |
| H_2O               | 8.5858              | NO                 | 0.0332              |
| N_2                | 2.8773              | CHO                | 0.0134              |
| HCl                | 5.2476              | O                  | 0.0154              |
| CO_2               | 0.9538              |                    |                     |

\[I_m = -6.09346 \times 10^5 \text{ cal}\]

\[G_m = -1.13375 \times 10^3 \text{ J}\]

\[T_c = 3634.4996 \text{ K}\]
4. Conclusions
Genetic algorithm based on descending dimension and mixture ranking not only effectively solves optimization of equilibrium ingredients with equality constrains, but also avoids recalculation caused by minus value, which is produced by using Lagrange multiplier method in engineering. Through calculation, propellant energy error between preburning and afterburning is only $6.56 \times 10^{-6}$, so the method’s accuracy is high. Moreover, there is no special requires for initial iteration parameters in this method, it is appropriate to calculate burning equilibrium ingredients for all types of propellant.

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