Research on Comprehensive Performance Optimization Method of Explosives and Propellants Oriented to the Whole Process

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Abstract. Explosives and propellants are common basic energy for weapons and equipment to achieve delivery, damage, and control, and are an important manifestation of national defense power. However, due to the wide variety of products and complex performance, the traditional serial design optimization mode can no longer meet the requirements of product diversification and rapid development. In this paper, the design process of explosives is deeply studied, and a method for optimizing the comprehensive performance of explosives and propellants oriented to the whole process is proposed. The method uses a comprehensive performance optimization engine to numerically model different design links in a unified parameter space, connects different links horizontally, and adopts a multi-objective optimization algorithm to comprehensively consider the optimization objectives of different links, realizing the automatic execution of the optimization process according to the design process. In order to verify the effectiveness of the method, this paper optimizes the formula of explosives and propellants based on two different types of explosives, gun propellant and rocket propellant. Experimental results show that this method improves the design efficiency and improves product quality under the premise of ensuring safety and manufacturability.

Keywords: Explosives and propellants; Optimization engine; Multi-objective optimization; parameter optimization.

1. Introduction

Explosives and propellants are generally composite energetic materials composed of oxidizers, combustion agents, high-energy explosives, and functional materials. They are the main energy sources for land, sea, and air weapons. They play an irreplaceable and important role in the fields of national defense and aviation. Due to the toxic reagents involved in the synthesis and production process and the products are flammable and explosive, the current design and development cycle of explosives and propellant is long and inefficient, which greatly limits the iterative update of explosive and propellant products. With the vigorous development of computer software and hardware technology, especially the aided design, the use of numerical simulation technology to carry out the proportion design, power calculation and damage effect analysis of explosives and propellants has gradually become a research hotspot in the field of explosives and propellants.

Foreign countries started early in the research of explosives and propellants. In terms of theoretical research, military powers such as the United States and Europe took the lead in adopting the research and development principle of " No experiment, Calculation first ". Since the 1970s, they have used advanced computer technology and combined structural chemistry, organic chemistry, quantum chemistry, physical chemistry, chemical informatics and other disciplines have carried out structural design, performance prediction, and virtual synthesis of explosives and propellants, effectively guiding synthesis experiments and greatly shortening the development cycle of new products, significantly reducing costs. In terms of simple energetic materials, the United States reduced the synthesis steps from four to three by calculating the synthesis mechanism of CL-20, so that the yield reached 92% and the purity was close to 100% [1]. Russia has done a lot of basic research work such as molecular design and route design on the furazan series of energetic materials, designed many energetic materials with excellent performance, and obtained the 3,4-bis. The new atom-economical

synthesis method of aminoglyoxime has become a new starting point for the synthesis of furan-like energetic materials. It is the first to synthesize bridged furan and furan-nitro compounds. The calculated detonation velocity of many compounds is close to 10000m /s [2]. In terms of mixed explosives and charges, a large number of researchers in the United States have been engaged in the research on the formulation and performance of explosives for a long time, and have established many effective theoretical models, such as the detonation model C-J model [3] and ZND model [4], and the non-ideal detonation model Wood-kirkwood model [5], BKW equation[6] and JWL equation[7] used to describe the state of detonation products, theoretical and empirical formulas used to estimate detonation parameters such as explosion pressure and detonation velocity[8], and the Forest Fire model [9], Lee-Tarver ignition growth model [10], JTF model [11], etc. used to simulate the shock safety of explosives, and the Cole and Zamyshlyayev empirical formulas used to calculate the explosion shock wave parameters of explosives in water, etc. [12], these Theoretical models and formulas are still used by explosives researchers all over the world and have played a huge role. Theoretical models are the basis for numerical simulations.

While using computer technology to improve design strategies and calculation methods, military developed countries have successively developed a variety of molecular design software for energetic materials [13]. For example, the LOTUSES software developed in India can realize the prediction of the detonation performance and thermodynamic properties of energetic materials, such as density, detonation velocity, detonation pressure, detonation heat, decomposition products, etc. The GenMolTM software developed in France uses structural parameters as descriptors to predict the impact and friction sensitivity of energetic materials. MATEO software can carry out the molecular design of energetic materials, and can realize the estimation of density, enthalpy of formation, detonation performance, etc. The thermochemical calculation software EXPLO5 developed in the Czech Republic can predict the density, enthalpy of formation, and detonation performance of energetic materials, and is also applicable to the prediction of combustion performance of metal composite energetic materials. The CHEETAH software for predicting the detonation performance of energetic materials developed in the United States has a rich database and is highly recognized in the industry. The RMG software predicts the reaction mechanism through molecular structure coding, combined with resources such as chemical databases, reaction rules, and online computational chemistry. Virtualization design has also been basically realized in the aspect of mixed explosive formula and charge design. For example, the United States already has a series of simulation design programs, which can simulate and predict the performance of certain formulations and charges in terms of energy, safety, and vulnerability. This means that the performance of the charge has been mastered before the range test is carried out, and the range test is only used as a final verification method.

Compared with developed military countries such as the United States, domestic theoretical research on explosives is still relatively weak, and basically stays in the analysis based on mature foreign theories, mainly focusing on the research on different attributes of explosives, focusing on the relationship between different attributes, there are few theoretical models and experimental methods independently proposed. For example, Wang Yawei [14] analyzed the influence of the relative content of components on the stability and safety of high-energy and low-sensitivity propellants. Zou Fengjuan [15] analyzed the extrusion time, extrusion temperature and extrusion die structure through numerical simulation to analyze the quality of the propellant. Zhao Liang [16] studied the effects of different sizes of ammunition on the cook-off response characteristics of explosives. Cheng Yuteng [17] studied the detonation shock wave characteristics of thermobaric explosives with different formulations in different environments through four methods: theoretical analysis, numerical simulation, open space static explosion test, and limited space static explosion test.

In terms of simulation programs, there are not many simulation calculation programs of explosives and propellants independently developed in China. Individual research teams use some software internally, such as flame sensitivity calculation, and tool software such as mechanical properties and

comprehensive sensitivity developed based on general commercial software. Although the software has been applied in the development of related products, there are still some problems: such as the independence of various objects, algorithm databases, etc., the lack of unified specifications, and the lack of unified calling; the software performance is unstable, poor compatibility, Complicated operations etc.

The performance of explosives and propellantsproducts is complex, and a large number of simulations and tests are involved in the design and development process. Although certain simulation technologies have been used in China, due to the particularity of the industry, many foreign software have blocked our country, resulting in the development of explosives is still mainly based on a large number of trial production tests, supplemented by simulation calculations. This research and development model relies heavily on experiments, resulting in high research and development time and economic costs; secondly, the existing model adopts the collaborative model of serial feedback and cannot meet the requirements of diversified and rapid product development. In order to meet the refined research and development under the new situation, it is necessary to carry out research on the comprehensive performance optimization of explosives and propellants, shorten the research and development cycle, and reduce the research and development cost. This paper studies the comprehensive performance optimization method of explosives and propellants, and proposes a comprehensive performance optimization method for explosives and propellants oriented to the whole process.

2. Comprehensive Performance Optimization of Explosives and Propellants

2.1. Design of comprehensive performance optimization engine

The development process of explosive and propellant products usually includes formula design, charge design, process design, quality design and other links, each link is closely related to the comprehensive performance of the product. At present, the traditional optimization idea is to decouple the research and development process, and to optimize the involved links or a single attribute, but the factors related to the performance of explosives are complex, and the whole process involves dozens of design and simulation analysis tool software, hundreds of items of manual and mechanical processes. The optimization process requires repeated iterations to carry out experimental verification. In this paper, a comprehensive performance optimization engine is used to unify a large amount of structured and unstructured data generated in the whole process of product development into the same parameter space, and carry out multi-objective optimization for the whole process to improve the comprehensive performance of explosives.

The optimization engine uses digital technology to carry out numerical modeling of each link in the development process, parameterizes the properties related to the performance of explosives, and solidifies the designer's experience knowledge and business rules into a model for rapid iteration. At the same time, the optimization engine learns the relationship between different links, opens up the data flow between different links, realizes process-based data linkage, greatly improves design efficiency, and achieves the purpose of automatic and full-process analysis.

Due to the particularity of explosives and propellants, it is necessary to coordinate and optimize performance indicators in different aspects under the control conditions of product safety and manufacturability constraints when carrying out comprehensive performance optimization and improvement. In this paper, machine learning methods are used to obtain performance evaluation models for different aspects of the product. Based on the comprehensive performance optimization algorithm library, a constrained multi-objective optimization method is used to build a comprehensive performance optimization engine for explosives and propellants that is oriented to the entire process. Based on the automatic intelligent analysis of the design process, the engine can assist designers to fully understand the design space of explosive and propellant products, and find the optimal solution according to the optimization goal. The overall framework is shown in Figure 1 below.

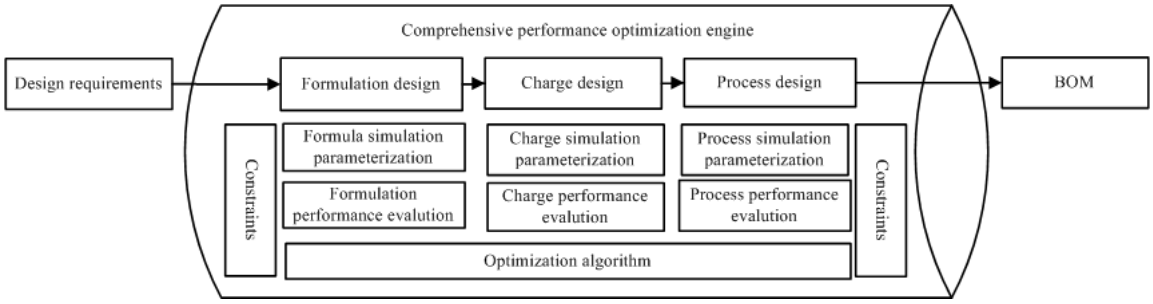

Fig. 1 The overall framework of comprehensive performance optimization engine

2.2. Multi-objective comprehensive optimization

As we all know, the purpose of optimization is to obtain a solution with the minimum cost from a problem that may have a large number of solutions, and avoid being trapped in a local optimum. Multi-objective optimization with constraints is usually a nonlinear problem, and simulated annealing algorithm is the most typical parameter optimization algorithm for finding the global optimal value in nonlinear problems.

The simulated annealing algorithm comes from the process of crystal cooling. In the world of molecules and atoms, the greater the energy, the less stable the molecules and atoms are. When the energy is lower, the atoms are more stable. If the solid is not in the lowest energy state, the solid is heated and then cooled. As the temperature drops slowly, the atoms in the solid are arranged in a certain shape to form a high-density, low-energy regular crystal, which corresponds to the global optimal solution in the algorithm. And if the temperature drops too fast, it may cause the atoms to lack enough time to arrange into a crystalline structure, resulting in an amorphous with higher energy, which is the local optimal solution. Therefore, according to the annealing process, the temperature of the object can be increased, and then cooled, and increasing energy can help jump out of the local optimal solution.

The simulated annealing algorithm is actually a greedy algorithm, but it introduces random factors in the search process. The simulated annealing algorithm accepts a solution that is worse than the current solution with a certain probability, so it is possible to jump out of the local optimum and reach the global optimum. The algorithm includes two parts, namely Metropolis algorithm and annealing process. In 1953, Metropolis proposed the importance sampling method, that is, to accept the new state by probability rather than using completely determined rules, which is called the Metropolis criterion, and the calculation amount is low. Metropolis algorithm is the basis of annealing to avoid the result falling into local optimum.

According to the Metropolis criterion, assuming the previous state is $x(n)$, the system changes to $x(n+1)$ according to a certain indicator state. Accordingly, the energy of the system changes from $E(n)$ to $E(n+1)$, and the acceptance probability P of the system changes from $x(n)$ to $x(n+1)$ is defined as:

$$P = \begin{cases} 1, & E(n+1) < E(n) \\ e^{-\frac{E(n+1)-E(n)}{T}}, & E(n+1) \geq E(n) \end{cases} \tag{1}$$

Where T represents the temperature. From the above formula, we can see that if the energy decreases, the transfer will be accepted. If the energy increases, it means that the system deviates farther from the global optimal value. At this time, the algorithm will not immediately abandon it, but carry out probability operation, where P determines the size of probability P by the amount of energy change and T, so this value is dynamic.

However, direct use of Metropolis algorithm may lead to too slow optimization speed. In order to ensure convergence in a limited time, it is necessary to set parameters to control the convergence of the algorithm. In the above formula, the parameter T can be adjusted. If the value of T is large, the annealing speed will be accelerated, and the iteration will end when the local optimal value is reached.

If the value is small, the calculation time will increase. Generally, the larger value of T is used at the initial stage of annealing, and will gradually decrease as the annealing proceeds. The formula is as follows:

$$T(n+1) = \lambda T(n) \tag{2}$$

Where, $T(n)$ represents the temperature at the nth round, $n = 1,2,3\cdots$, where λ is a positive number less than 1, and the value is generally between 0.8 and 0.99.

3. Experiments

On the basis of in-depth research on the comprehensive performance optimization of explosives and propellants, with the help of rapid packaging and integration technology, this paper constructs a comprehensive performance optimization engine that covers the input and output of standardized parameters and is oriented to the entire process of explosives and propellants. In order to verify the optimized engine performance, experiments were carried out based on two types of explosive and propellant.

3.1. Experimental setup

There are many types of explosives, and different product development and design processes are different, resulting in differences in optimization steps. Comprehensive performance optimization needs to design different processes for different types of explosives and propellants, then parameterize each link, and finally carry out optimization under a unified framework.

3.1.1 Process creation

The comprehensive optimization engine includes all possible links in the design of explosives and propellants, achieving full coverage of the research and development process of explosives and propellants. A process template can contain several process nodes. The logical sequence relationship between nodes can be automatically generated with the help of big data analysis technology and supports custom modification. The input and output data of nodes and node trigger conditions can be adjusted as needed, as shown in Figure 2 shown.

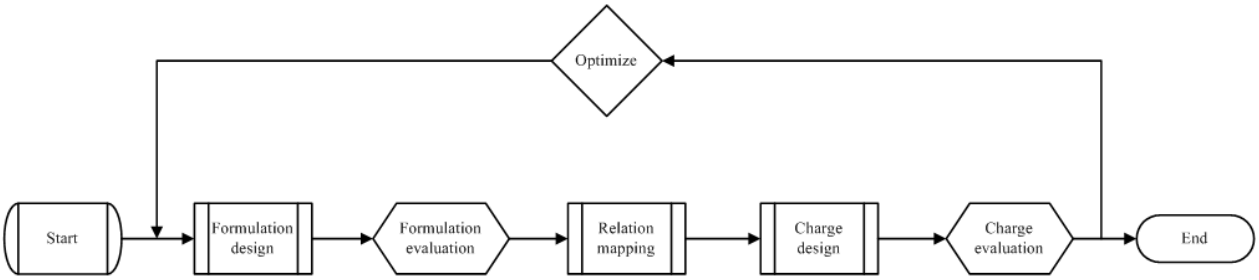

Fig. 2 Examples of processes created in the optimization engine

3.1.2 Model parameterization

The optimization engine uses big data analysis technology to analyze the impact of various factors on the comprehensive performance, mines the correlation between data, and automatically builds the correlation between the input and output parameters of different modules, so as to realize the automatic iterative optimization of the optimization process according to the business process.

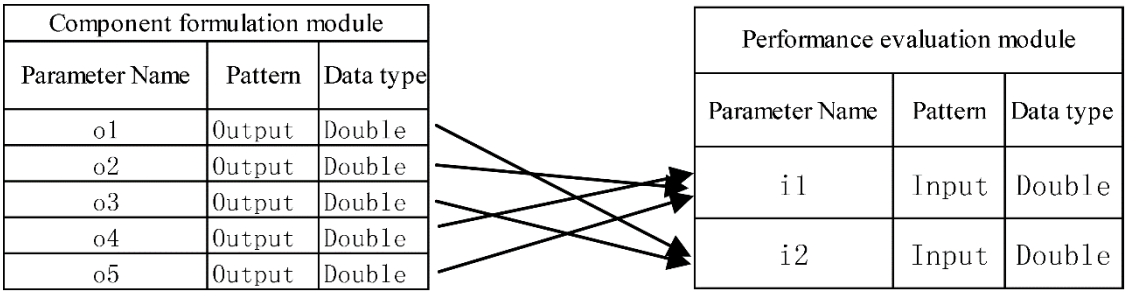

Fig. 3 An example of the relationship between the inputs and outputs of different modules in the optimization engine

3.1.3 Optimization process

On the premise of the safety and manufacturability of explosives and propellants, the optimization engine optimizes the composition ratio to improve product performance according to the different design requirements of gun propellants and rocket propellants.

In the experiment, the component distribution ratio is used as input data, and the upper and lower limits of the component distribution ratio are used as the key factors affecting the safety and manufacturability of explosives and propellants, and the optimal solution is obtained from a large number of possible solutions at the minimum cost.

In the experiment, the group allocation ratio is taken as the input data, and the upper and lower limit of the group allocation ratio is taken as the key factor affecting the safety and manufacturability of explosives, and the optimal solution is obtained from a large number of possible solutions at the minimum cost. The optimization process takes the explosion temperature value of the gun propellant and the specific impulse of the rocket propellant as constraints, and optimizes the composition ratio so that the gunpowder power of the gun propellant and the temperature of the rocket propellant are close to the expected target. In order to avoid falling into a local optimum, the simulated annealing optimization algorithm in the optimization algorithm library was selected for optimization in the experiment.

3.2. Experimental results

The maximum temperature parameter of the simulated annealing algorithm is set to 1000, the minimum temperature is 100, the annealing rate is 0.8, the number of iterations in each round is 30, the probability coefficient is 100, and the retrieval step is 3. In the optimization process, the Energy software is used to calculate the energy by using the calculation method of constant energy and constant volume. The composition ratio in the formulation design of explosives and propellants is used as the input parameter of the optimization engine, and the upper and lower limits corresponding to different parameters are shown in Table 1 below.

Table 1. The upper and lower limits of different components in the formulation design of propellants

Numble	Component Name	Parameter Name	Component Upper Limit	Component Lower Limit
1	Ingredient1	A1	10	0
2	Ingredient2	A2	25	0
3	Ingredient3	A3	25	0
4	Ingredient4	A4	25	0
5	Ingredient5	A5	100	0

In the gun propellant experiment, the detonation temperature value is a constraint condition, represented by Y1,, set to 3500k, the deviation must not exceed 20%, that is, the temperature results between 2800k~4200k meet the requirements, the number of cycle constraints is 100, and the

maximum cycle time for 10 seconds. The gunpowder power is the optimization target variable, and the expected target value is 1350J/Kg, denoted as M1.

In the rocket propellant experiment, the specific impulse value is used as a constraint condition, represented by Y2, which is set to 2600s, and the deviation must not exceed 20%, that is, the result of the specific impulse between 2470s and 2730s meets the requirements. The target variable of propellant detonation temperature optimization is denoted by M2, and the expected target value is 3500k.

Observing the optimization process of the comprehensive performance optimization engine, it can be found that in the gun propellant experiment, the value of the propellant power gradually converges to around 1260, as shown in Figure 4; when the component ratio is set to 5:15:1:21:58, the gunpowder power of the gun propellant is closest to the expected value of 1350, as shown in Table 2 below. At this time, the gunpowder power value is 1260.71, and the explosion temperature is 3353.15. In the rocket propellant experiment, the detonation temperature gradually converges to around 3380, as shown in Figure 5; when the component ratio is 4:8:0:2:86, the detonation temperature is closest to the expected value of 3500, as shown in Table 3 below Show, At this time, the explosion temperature value is 3384.47, and the specific impulse is 2631. The experimental results show that the comprehensive performance optimization engine can optimize the ratio design of explosives and propellants, quickly find out the optimal design scheme, improve the efficiency and product quality of explosive and propellant development, and prove the effectiveness of the method in this paper.

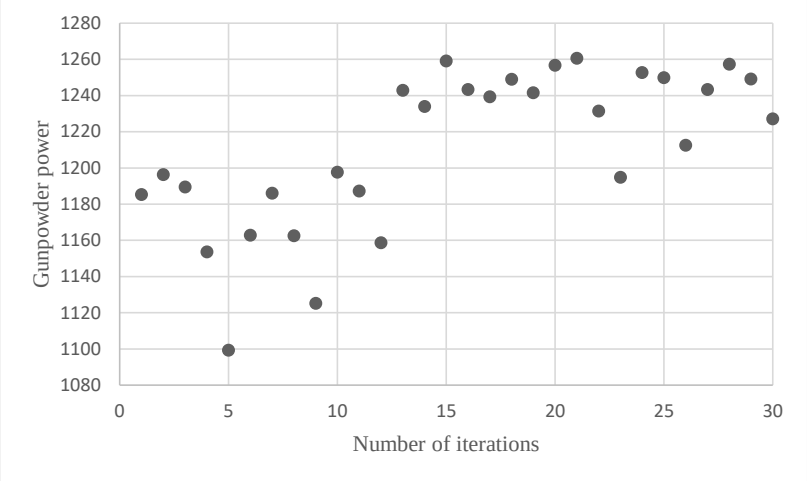

Fig. 4 The change process of gun propellant force value in optimization process

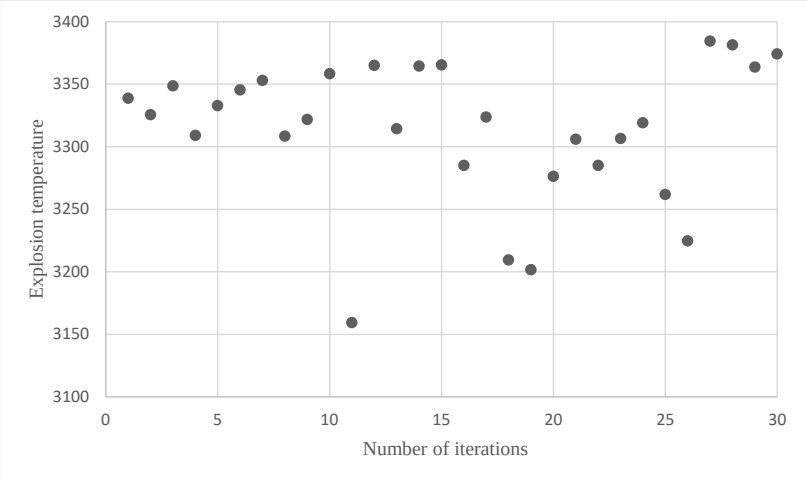

Fig. 5 The change process of rocket propellant detonation temperature in optimization process

Table 2. Experimental results of gun propellant

DesignID	A1	A2	A3	A4	A5	Y1	M1
1	4	2	12	8	74	3231.38	1185.29
2	1	5	5	5	84	3609.62	1196.3
3	6	4	8	0	82	3572.57	1189.57
4	6	2	4	2	86	3617.81	1153.71
5	4	4	0	0	92	3609.83	1099.35
6	2	8	0	4	86	3668.84	1162.94
7	6	4	6	2	82	3599.31	1186.17
8	2	6	4	0	88	3637.19	1162.66
9	0	8	0	0	92	3642.99	1125.27
10	6	6	0	10	78	3658.25	1197.76
11	1	7	1	7	84	3662.13	1187.25
12	7	1	3	5	84	3619.31	1158.73
13	3	9	1	15	72	3586.92	1242.88
14	8	6	2	18	66	3467.62	1233.99
15	8	12	0	20	60	3459.62	1259.12
16	3	15	3	21	58	3230.08	1243.45
17	5	15	3	21	56	3207.00	1239.33
18	3	13	3	19	62	3332.20	1248.99
19	11	15	1	23	50	3215.27	1241.66
20	9	17	1	21	52	3279.80	1256.78
21	5	15	1	21	58	3353.15	1260.71
22	0	10	6	16	68	3300.83	1231.52
23	8	10	6	20	56	3056.64	1194.95
24	6	12	2	18	62	3414.25	1252.81
25	2	10	2	16	70	3522.35	1249.89
26	6	12	6	18	58	3126.86	1212.59
27	2	10	4	16	68	3412.18	1243.38
28	10	12	0	16	62	3545.03	1257.34
29	8	10	0	16	66	3574.05	1249.14
30	4	12	6	16	62	3226.52	1227.2

Table 3. Experimental results of rocket propellant

DesignID	A1	A2	A3	A4	A5	Y2	M2
1	3	3	3	3	88	2607.1	3338.83
2	1	1	1	1	96	2582.3	3325.71
3	3	3	1	1	92	2602.9	3348.7
4	0	0	0	2	98	2562.9	3309.21
5	0	2	2	0	96	2593.6	3333
6	6	4	2	4	84	2609.6	3345.43
7	2	6	2	4	86	2617.7	3353.13
8	5	5	5	1	84	2596	3308.57
9	3	5	3	5	84	2601.7	3321.84
10	5	7	1	5	82	2619.9	3358.43
11	8	8	4	8	72	2547.7	3159.43
12	4	4	0	4	88	2616.4	3365.21
13	3	7	3	5	82	2601.9	3314.51
14	5	5	1	3	86	2619.3	3364.57
15	1	7	1	5	86	2624.8	3365.47

16	4	8	4	4	80	2592	3285.17
17	4	6	4	2	84	2604.3	3323.76
18	2	8	4	8	78	2565.6	3209.56
19	0	10	4	8	78	2568.1	3201.73
20	4	4	4	6	82	2580.7	3276.46
21	2	6	4	4	84	2597.3	3306.1
22	4	8	4	4	80	2592	3285.17
23	4	10	4	2	80	2604.4	3306.77
24	0	4	4	4	88	2600.6	3319.15
25	4	6	4	6	80	2579.1	3261.93
26	0	8	4	8	80	2571.3	3224.71
27	4	8	0	2	86	2631	3384.47
28	5	9	1	1	84	2632.7	3381.43
29	7	5	1	3	84	2618.4	3363.76
30	3	7	1	1	88	2625.8	3374.28

4. Summary

As the basis of energetic materials, explosives and propellants have complex manufacturing processes and product properties. The traditional serialization optimization method is to optimize each link in the design process separately, the optimization efficiency is low, and the operation is cumbersome. This paper deeply analyzes the design process of explosives and propellants, and proposes a comprehensive performance optimization method for explosives and propellants oriented to the whole process. The method uses a comprehensive performance optimization engine to numerically model the different design links of explosives and propellants, open up the data links between different links, unify the design of explosives and propellants into the same parameter space, and then optimize the results based on multi-objective optimization. In order to verify the effectiveness of the method, this paper carried out formula optimization experiments based on two different types of explosives and propellants. The results show that the comprehensive optimization engine can improve the design efficiency and quality of explosives and propellants on the premise of satisfying the safety and manufacturability, and achieve the goal of reducing the test cost and shorting development cycle.

Acknowledgements

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