Meso-model Optimization of Composite Propellant Based on Hybrid Genetic Algorithm and Mass Spring System

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Abstract. The meso-structure of composite propellant directly affects its macroscopic properties. The primary premise of studying the macroscopic characteristics of composite propellant is to establish the meso-structure model which can reflect the actual formulation characteristics. In order to obtain the optimal composite propellant meso-structure model suitable for numerical analysis and calculation, the hybrid genetic algorithm was used to optimize the reconstructed meso-structure model. In order to avoid different degree of overlap between particles, the mass spring system was further improved. The resulting meso-structure model not only preserves the statistical characteristics of the propellant, but also meets the requirement of minimizing the optimal size. The reconstruction and optimization algorithm of the optimal meso-structure model are established in this paper, which has high theoretical significance and engineering application value for the prediction of mechanical properties of composite propellant.

Keywords. Meso-model optimization; composite propellant; hybrid genetic algorithm.

1. Introduction
Composite propellant is a kind of special particle reinforced composite material. It is a multi-component system in composition. There are two phases: matrix phase composed of binder matrix and particle phase composed of inorganic oxidant and metal aluminum powder. With the development of computer technology, the application of computer simulation and numerical calculation technology to the numerical analysis of composite propellant can not only reduce the development cost but also make up for the shortage of actual material design and preparation, which provides scientific guidance and theoretical basis for the formulation design of composite propellant [1].

The meso-structure of composite propellants is characterized by large number of particles, large size difference and diverse shapes. How to mathematic describe the geometrical shapes of the meso-structure as well as the numerical reconstruction and reproduction of the meso-structure has always been the focus and difficulty of the current research. In order to be able to represent the actual propellant materials, the geometrical model generated by the computer must be large enough. For the composite propellant with high volume fraction, the numerical analysis efficiency is very low due to the large amount of calculation, and the practical application value is not high. Therefore, it is very important to apply the optimization technology to solve the size problem under the premise of keeping the statistical characteristics of the propellant meso-structure unchanged. Based on the representative element optimization method, in view of the particle volume fraction is high, the shape of diverse requirements, combined with the common advantages of genetic algorithm and simulated annealing
algorithm, through repeated iteration, constantly adjust the RVE particle coordinates, but between particles could be for different degree of overlap, mass spring system is effectively to avoid the overlapping. Finally, the optimal cell geometry model is generated to meet the requirements [2].

2. Meso-model Optimization Design Based on Hybrid Genetic Algorithm and Mass Spring System

The generation process of cellular model is divided into two stages. The first stage is to use hybrid genetic algorithm to greatly reduce the number of particles in the original cellular model input. The second stage is to optimize the reduced cellular model to eliminate the possible overlap of particles.

2.1. Hybrid Genetic Algorithm

Hybrid genetic algorithm is an intelligent algorithm for optimization problems. It combines the common advantages of genetic algorithm and simulated annealing algorithm, that is, it has fast convergence speed and good optimization effect, and has different application space for different practical problems. In this paper, hybrid genetic algorithm is applied to the micro-structure optimization of composite propellant. Its flow chart is shown in figure 1, and the specific process is as follows [3].

Algorithm flow:
Step1: Given the evolutionary algebra counter gen, the initial temperature T and the maximum number of evolution maxgen;
Step2: Determine the coding scheme and randomly generate the initial population P0;
Step3: Construct the fitness function and calculate the fitness value of the population;
Step4: Introduce the optimal retention strategy, and completely copy the individual with the highest fitness in the current population to the next generation population Pt;
Step5: Conduct genetic operations such as selection, crossover and mutation on the new population;
Step6: Use the Metropolis rule, and insert Pt in the new entity;
Step7: gen=gen+1, if gen<maxgen, return Step5;
Step8: T=T*0.999, if the minimum temperature is not reached, go back to Step5;
Step9: Decode the optimal solution obtained by genetic algorithm.

2.2. Mass Spring System Optimization

For the cell model with small volume fraction, the number of particles is relatively small, so the above algorithm can solve the problem of particle overlap, however, when the submitted fraction is more than 60%, it is difficult to solve the poor overlap through the above algorithm. In this paper, the mass spring system is used to further solve this problem. In the micro-structure of particle cell, the overlapping phenomenon only occurs between a certain particle and its surrounding particles [4], therefore, Delaunay triangulation is constructed between adjacent particles, and the node is the center of the particle. In order to eliminate the overlap, it is assumed that there is a mass spring between each node in Delaunay triangulation [5, 6], and only the adjacent particles in the same Delaunay triangle can interact with each other. For a pair of overlapping particles, a hard repulsive spring is introduced to push the particles away from each other. For a pair of non-overlapping particles, a soft attraction spring is introduced to keep the particles close to each other, which will not lead to a new operator that will make a big change in statistical characteristics. It is further assumed that the mass of a particle is proportional to its volume. According to the standard spring dynamics, the following motion equation is constructed:

\[ M + Ku = 0 \]  (1)

where \( u \) is granular displacement vector, \( M \) is spring mass matrix, \( K \) is full strength matrix, and both \( M \) and \( K \) are diagonal matrices. The original state displacement is given by the original spring excitation caused by the overlap. Original displacement vector is:
\[ u_i = \frac{1}{2} \left[ \sum_{i=2}^{N} d_{i1}, \sum_{i=2}^{N} d_{i2}, \cdots, \sum_{i=2}^{N} d_{iN} \right]^T \]  

(2)

where \( N \) is the number of granular, \( N_i \) is the number of particles adjacent to the particle \( i \), \( d_{ij} = L_{ij}(\cos(\theta_{ij}), \sin(\theta_{ij}))^T \), \( L_{ij} \) is the overlap length of the particles \( i \) and \( j \), \( \theta_{ij} \) is the Angle between \( L_{ij} \) and the horizontal direction. In order to find out the moving distance of \( K \) and \( M \), each particle in the direction of \( Y \) and \( X \) are constructed as follows:

\[ M = \frac{1}{2} \text{diag} \left\{ \sum_{i=2}^{N} L_{i1} \cos \theta_{i1}, \sum_{i=2}^{N} L_{i1} \sin \theta_{i1}, \cdots, \sum_{i=2}^{N} L_{i2} \cos \theta_{i2}, \sum_{i=2}^{N} L_{i2} \sin \theta_{i2} \right\} \]  

(3)

\[ k_i = \left( \sum_{i=2}^{N} L_{i1} \cos \theta_{i1} + \sum_{i=2}^{N} L_{i2} \sin \theta_{i2} \right)^2 \]  

(4)

\[ K = \text{diag} \{ k_1, k_1, k_2, k_2, \cdots, k_N, k_N \} \]  

(5)

The dynamic equation of mass spring system is solved implicitly by standard Newmark [7].

**Figure 1.** Flow chart of hybrid genetic algorithm.
3. Based on GA’s PUC Mesostructure Reconstruction

3.1. Meso-structural Geometric Model
Because the number of particles is too large and the calculation efficiency of numerical analysis is too slow [7], the two-dimensional single-dimensional round particles are taken as the research object, the body integral number is 50%, the particle diameter is 100 μm, the original cell model has a dimension of 970 μm × 970 μm.

(a) Original cell  
(b) Optimal meso-characteristic cell

Figure 2. Comparison diagram of meso-cell model after optimization.

Figure 2a shows the comparison of the optimized meso-statistical features. In order to get the precise minimum size, under the advance of the error range of particle body integral, the best meticulous cell in the past is optimized again, and the dimension of the best meticulous cell in the end is 436.725 μm × 436.725 μm including 12 particles. Figure 2b shows the comparison of meso-statistical characteristics after re-optimization. It can be found that the size of the best meso-characteristic cell is about 1/5 of that of the original cell. Figure 3 is the mesoscopics statistics feature comparison chart, We can see that the statistical characteristics of the two probability functions are very close to each other, so the optimization model can replace the original model [8, 9].

Figure 3. Comparison of meso-statistical characteristics.

3.2. Numerical Analysis Calculation Model
At this time, the established meso-geometric model does not contain any mechanical characteristics, and the stress analysis can only be carried out after it is endowed with real material properties. Component parameters of elastic composites are given in table 1.
Table 1. Component parameters of elastic composites.

| Component | Diameter (um) | Modulus (MPa) | Poisson’s ratio |
|-----------|---------------|---------------|----------------|
| Substrate | —             | 1             | 0.49           |
| Particles | 100           | 32,450        | 0.14           |

Mesh division is a necessary condition for mechanical calculation of composite materials, and the shape, size and quality of mesh directly affect the mechanical calculation results. In order to simplify the calculation, this chapter adopts uniform quadrilateral mesh. In Abaqus 6.11 finite element analysis, the mesh division of the original cell and the best characteristic meso-cell is shown in figure 4, and the maximum size of the mesh is about 1/11 of the diameter.

![Figure 4. Quadrilateral meshing.](image)

(a) Original cell grid  
(b) Optimal cell grid

It can be seen from figure 4 that due to the relatively large number of particles in the original meso-cell, when the distance between the particles is very close, the grid density is not very uniform; However, due to the small number of particles, the distance between particles is relatively sparse, and the grid density is excessive and uniform, the overall effect is better.

Under the same meshing conditions, stress loads are applied to them respectively. According to the direction of action, stress can be divided into tension and pressure, in order to analyze the stress-strain relationship, horizontal and rightward tension is added to the original cell and the best meso-characteristic cell, with a load of 0.1 MPa, the stress distribution is shown in figure 4, and the right side of the model is fixed, under the action of tension, the meso-model will generate displacement strain to the right.

3.3. Analysis of Calculation Results

The deformation of the meso-model under stress is called strain. Figure 5 shows the macro stress-strain curve corresponding to the meso-model, in which both stress and strain are average values. Table 2 shows the relative error after calculation. The relative error of stress-strain curve between the original cell and the best meso-characteristic cell is less than 2%. Therefore, it can be concluded that the best meso-cell can completely replace the original cell as a complete structure and be applied to the macro-performance research of composite materials.
Figure 5. Statistical diagram of stress-strain.

Table 2. Comparison of stress-strain errors.

| Strain (%) | 0.010 | 0.015 | 0.020 | 0.025 | 0.030 | 0.035 |
|------------|-------|-------|-------|-------|-------|-------|
| Original cell stress (MPa) | 0.0288 | 0.0424 | 0.0559 | 0.0695 | 0.0822 | 0.0949 |
| Optimum cell stress (MPa)   | 0.0279 | 0.0415 | 0.0542 | 0.0678 | 0.0805 | 0.0932 |
| Relative error (%)          | 0.347  | 2.122  | 3.041  | 2.446  | 2.068  | 1.791  |

4. Conclusion

Study on optimization method of composite propellant meso-structure model. In order to generate the best meso-structure model of composite propellant suitable for numerical analysis and calculation, the reconstructed meso-structure model is optimized by using hybrid genetic algorithm. In view of the overlapping phenomenon between particles that may occur in the optimization process, the mass spring system is established to eliminate it. In order to improve the efficiency of the algorithm, a parallel optimization algorithm based on CPU+GPU hardware architecture is designed and implemented, and an ideal speedup ratio is obtained. The meso-structure model obtained by the optimization algorithm not only retains the statistical characteristics of propellant, but also meets the requirements of minimizing and optimizing the size [10].

The reconstruction and optimization algorithm of the best meso-structure model established in this paper has high scientific theoretical significance and engineering application value for the prediction of mechanical properties of composite propellants, and has important reference and guiding role for the formulation design of propellants and measures to improve mechanical properties. The research method in this paper has strong universality and can be extended to the application of other particle reinforced composites such as concrete, sand, rock and soil.

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