Composition design of Nickel-Based Superalloy Based on Data-Driven Methods in Investment Casting

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Abstract: Investment casting has been widely applied to fabricate aircraft due to its high dimensional accuracy and excellent surface finish with complex geometries. However, defects such as shrinkage porosity and misrun often occur in these castings. Traditional trial-and-error procedure have hindered the application of investment castings in high-end applications. In this research, a novel data-driven approach for predictive modeling is proposed to address these challenges. With integrated computation of thermodynamic and finite element method (FEM), a variety of components within the boundary of Ni-based superalloy K4169 were evaluated for both fluidity and shrinkage with two patterns. A numerical model incorporating machine learning algorithms was developed based on the integrated computation. For K4169 superalloy castings, the shrinkage porosity is primarily influenced by Al element, while misrun is mainly correlated with Al, Ti, and Mo in a decreasing order. This data-driven model establishes a quantitative relationship between composition and final product defects. The method proposed in this study shows promise for optimizing the investment casting process and can be applied to a wide range of alloys and models.

Keywords: Integrated computation, Data-driven approach, Ni-based superalloy, Investment casting

1 Introduction

Investment casting is a precise forming technique applied in advanced fields such as aerospace, for its intricate design capabilities and high-quality finish.[1] However, the reliance on traditional trial-and-error approaches in the research and development phase often results in huge waste.[2] The introduction of data modeling and big data algorithms has significantly improved the efficiency of the investment casting process. By incorporating advanced computational techniques such as machine learning algorithms and predictive modeling, manufacturers can analyze extensive datasets to identify optimal casting parameters and predict casting defects with enhanced precision.

With great tensile strength, hardness and fatigue life, Ni-based superalloy has been widely applied in aerospace castings. However, the composition of certain superalloy varies in a large bound, which leads to significant uncertainty in properties such as liquidus, solidus and fluidity. These properties contribute to the formation of casting defects, so this uncertainty can lead to misprediction. In this research, to address the challenge of composition induced casting defects, a data-driven framework is proposed. The schematic is shown in Figure 1.

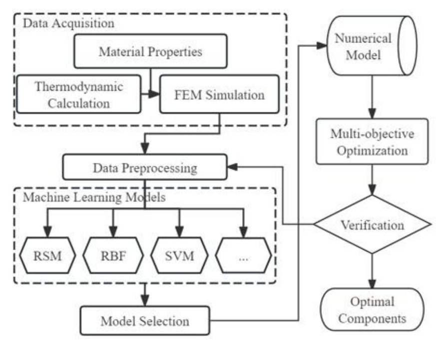


Figure 1. Data-driven framework of this research

2 Experimental procedure

In this research, K4169 Ni-based superalloy is taken as the experimental alloy. Its nominal composition is shown in Table 1.

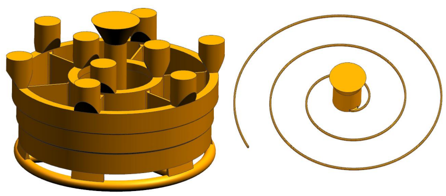
Table 1. Nominal composition of K4169 superalloy

Elements	Al	Cr	Ni	Fe
Lower bound (wt%)	0.30	17.00	50.00	Bal.
Upper bound (wt%)	0.70	21.00	55.00	
Elements	Mo	Nb	Ti	
Lower bound (wt%)	2.80	4.4	0.65	
Upper bound (wt%)	3.30	5.4	1.15	

The performances of different alloy compositions within the limit of K4169 is calculated with Pandat Ni-database. Optimal Latin hypercube sampling was utilized to develop a more effective numerical model. 100 sets of compositions are designed with Latin hypercube sampling, and their performance are calculated with high-throughput calculation in Pandat software.

Compositions and their performance are imported into database. Featured patterns in Figure 2 are designed to address shrinkage porosity and misrun defects. FEM calculations are carried out with ProCAST software. Results are automatically extracted from calculated files.

To establish the relationship model between components and performance, different machine-learning algorithms are applied to the result. In this research, RBF, RSM, linear regression and SVR are applied. The data is divided into training set, validation set and test with a ratio of 2:1:1, and then approximated with the models above.



(a) Shrinkage (b) Misrun

Figure 2. Featured patterns

3 Result and discussion

Composition-performance-defect numerical model

The comparison of different machine learning models is shown in Figure 3. In almost all properties in performance, microstructure and defect, RSM algorithm shows the best coefficient of determination. Numerical model is established with RSM algorithm. The correlation table between composition and properties is shown in Table 2.

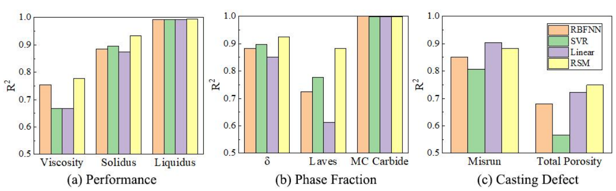
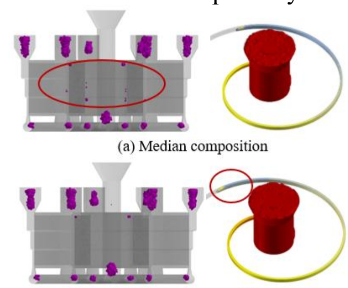


Figure 3. Coefficient of determination among different algorithms

Table 2. Composition-performance-defect correlation table

Elements	Al	Cr	Fe	Mo	Nb	Ti
Misrun	-0.54	0.07	0.03	-0.32	-0.09	-0.45
Porosity	0.79	-0.05	0.05	-0.28	-0.26	-0.39

3rd generation non-dominated sorting genetic algorithm (NSGA-III) is applied to the component optimization. After 40 generations of iteration, the optimal component is: Al 0.79%, Cr 18.1%, Fe 20.1%, Mo 3.08%, Nb 5.25%, Ti 1.09%. Simulation verification in Figure 4 indicates that the optimal compositions is enhanced with 23% less internal shrinkage and 13% increased feed length, compared to median composition of K4169 superalloy.



(a) Median composition

(b) Optimal composition

Figure 4. Numerical verification of optimal composition

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5 Conclusion

In this research, machine learning algorithms is combined with thermodynamic-FEM integrated computation to develop the numerical model. The NSGA-III algorithm is then applied to optimize the components based on the model. The following conclusions can be made:

a) Within the boundary of K4169 superalloy, shrinkage porosity is primarily influenced by Al, while misrun is negatively correlated with Al, Ti and Mo.
b) The optimal composition within K4169 limit has 23% less internal shrinkage and 13% increased feed length in featured patterns, compared to median.
c) The data-driven approach proposed in this research shows promise in deviation analysis and composition optimization.

References

[1] L. Liu, The progress of investment casting of nickel-based superalloys. J. Foundry, 2012, 12: 1273-1285.
[2] Wang D, Sun F, Shu D, et al. Data-driven design of nickel-based casting superalloys and precise forming of complex castings. J. Acta Metallurgica Sinica, 2022, 58(1): 89-102.