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Computer-Aided Design and Applications

Predicting Die Cracking in Die-Cast Products Using a Surrogate Model Based on Geometrical Features

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Abstract. This paper explores the development and application of a surrogate model for predicting die cracks in die-cast products, focusing on the geometrical features of the product design. Die casting, a method renowned for its efficiency in rapidly producing complex shapes, is particularly significant in the automotive industry in reducing vehicle weight and part count. However, ensuring product quality and minimizing development lead time remain critical challenges exacerbated by difficulties in predicting defects in complex shapes at the product design stage. Traditional simulation technologies, while standard, are limited by long preparation and execution times, prompting a shift towards utilizing big data and machine learning for more efficient defect prediction. This study introduces a novel surrogate model that employs Variational Autoencoders (VAEs) and neural networks to predict the occurrence of die cracks, a pressing issue in die-casting that can lead to significant production delays and costs. By analyzing engine block parts and transaxle cases from Toyota Motor Corporation, the model demonstrates promising results in predicting die cracks with high accuracy. The findings suggest a new direction for improving the die-casting process, leveraging product shape data for early defect detection, thereby enhancing manufacturing efficiency and product quality.

Keywords: Die casting, Surrogate model, VAE, Neural network, Computer-aided design, die cracking, geometrical features, automotive industry, machine learning, defect prediction, 3D shape data
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1 INTRODUCTION

Die casting is widely used in industrial production because it mass-produces products with complex shapes at high speed. Especially in the automotive industry, die casting has attracted renewed attention in recent years from the viewpoint of vehicle weight reduction and reduction of the number of parts in products, e.g. [1]. To ensure high competitiveness as an industrial product, it is necessary to supply products that correctly reflect market trends on time, and for this purpose, it is crucial to shorten the lead time for product development.

Usually, the product development process in the automotive industry follows the flow below:

Product design ⇔ Die design ⇔ Productivity simulation ⇔ Process design ⇔ Functional evaluation ⇔ Mass production

This process is not unidirectional but iterative, enhancing the completeness of the product design through repeated cycles of each step. However, as the process advances, the specifications become more complex, and corrections or rework tend to increase. Therefore, it is crucial to proceed with as few reworks as possible.

To reduce the number of reworks and shorten the product development lead time, it is essential to achieve a high-quality design that considers not only the product shape but also material selection and the development of a manufacturing plan from the early stages of product design. According to best practices as stated by Pahl and Beitz [2], product design must encompass these aspects to ensure the final product meets all necessary criteria. However, it is often challenging to make accurate predictions for products with complex shapes in the initial design stages, and this can lead to rework if these factors are not adequately considered early in the design process.

In this context, a "pre-prediction" refers to a preliminary estimation of potential defects during the early design stages. This differs from a detailed prediction, which is conducted in the subsequent design phases. Accurate pre-predictions are challenging for products with complex shapes, and inaccuracies at this stage can contribute to the need for rework.

2 LITERATURE REVIEW

2.1 Simulation Technology in Industrial Product Development

One way to solve this problem is to predict the functionality using simulation before manufacturing the product and rectifying issues beforehand. Indeed, simulation technology is widely adopted and has become a standard technique in industrial product development processes [3, 4, 5, 6]. Efforts are also ongoing to enhance accuracy, for instance, in casting simulation, traditionally focusing on fluid analysis of molten metal, but now also incorporating calculations for ambient air compression behaviors to examine the back pressure influences and improve accuracy regarding splashing behaviors at the spout [7]. Additionally, research is being carried out to reduce computation time using quantum computers to speed up the examination cycle [8]. However, even if these technologies are put into practical use, preparing model information of the die for manufacturing is necessary to execute a simulation. Including revisions, it takes several days to complete a simulation once. Therefore, even if improvements in simulation accuracy and time reduction are realized, only part of the problem of long preliminary examination time utilizing simulation is solved, leaving the challenge of easy defect prediction in the early stages of product development unresolved.

2.2 Limitations of Current Simulation Techniques

Given these limitations with simulation technology advancements, an alternative approach is actively pursued, which involves analyzing and utilizing big data obtained from defect occurrence information of manufactured products in the past and accumulated simulation results to convert pattern recognition into added value for current and future productivity predictions [9]. Among these efforts, the technique known as surrogate modeling, which employs machine learning or other methods to predict using patterns obtained from known data instead of executing detailed simulations, is gaining traction as it enables the reduction of computation costs and pre-required information. For instance, Amir Pouya proposed a model capable of predicting the cross-sectional temperature distribution of the welding pool by learning laser welding processing parameters using a neural network [10]. Additionally, Andres and others reported the effectiveness of a predictive model utilizing SVM as a means to estimate the cross-sectional shape of aircraft blades at a low computation cost [11]. Therefore, surrogate models, performing necessary predictions with reduced, original information based on known data, are likely to solve the problem of accurately predicting product quality from product shape in the early development stages. However, many of the cases reported so far simplify the problem by reducing three-dimensional phenomena to two dimensions, and it needs to be clarified whether it can be directly applied to phenomena where complex three-dimensional shapes are the subject of prediction. Also, there are very few reports on the effectiveness of surrogate models for defect occurrence in the casting process based on the geometric information of the product. If the possibility of realization is shown, it significantly impacts the industrial product development process.

2.3 Big Data and Surrogate Modeling

In our previous research [12], we reported the successful development of surrogate models for predicting soldering defects in die-cast products using a Variational Autoencoder (VAE) [13] and Neural Network (NN). Variational Autoencoders (VAEs) are a class of deep learning models that have gained attention for their ability to learn efficient representations of data in an unsupervised manner. Unlike traditional autoencoders, VAEs impose a probabilistic structure on the latent space, which allows for generating new data points that are similar to the training data. This characteristic makes VAEs particularly useful in applications where data augmentation and anomaly detection are crucial. In the context of manufacturing, VAEs can be leveraged to predict defects by learning from historical data and identifying patterns that signify potential issues. This technique not only enhances the accuracy of predictions but also reduces the computational burden associated with traditional simulation methods.

This notably contributed to the improvement of the development process, especially by enhancing prediction accuracy during the product design phase. However, the effectiveness of this approach for predicting other types of defects that may arise during the die-casting process, particularly cracks in dies, has not yet been confirmed.

This paper details the development process of the die crack prediction model, the data set used, the methods of accuracy evaluation, and the results obtained, proposing new directions for the improvement of the die-casting process.

3 TARGET FAILURE

Die cracking, which refers to cracks in the casting die caused by thermal stress, is illustrated in Figure 1. This thermal stress arises from non-uniform thermal expansion or contraction resulting from temperature changes within an object. The occurrence of thermal stress is largely dependent on the material properties, the rate of temperature change, and especially the shape of the object.

The impact of shape on thermal stress is significantly important, especially in areas where thermal expansion is severely constrained, such as corners or fine details, leading to pronounced stress concentration due to shape. Additionally, the heat supplied by the contacted molten metal contributes to the temperature rise, but the amount of heat received per volume of the die depends on the contact area, the thickness of the cast product, and the volume of the die, indicating a substantial impact of shape factors in this aspect as well.

Given this background, attempts to predict die cracking based on the characteristics of the product shape are considered valid. Therefore, it has been selected as a target defect for prediction using surrogate models.

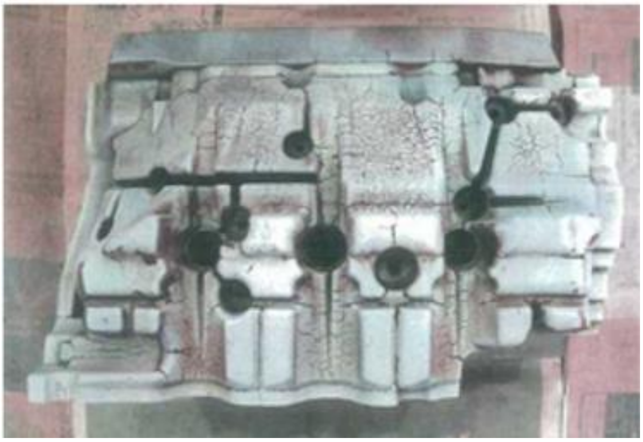

Figure 1: Image of Die in the actual die-casting process, which has cracks (red lines) on the surface.

4 DATASET AND ANALYSIS TARGET

4.1 Simulation of the Prediction Target

Metal fatigue failure progresses exponentially with the number of cycles of repeated stress. Additionally, in die-casting processes, die cracking, which is a major issue, often occurs due to low-cycle fatigue. Reference [14] sets the number of cycles at 20,000 shots to evaluate the fatigue strength of various hot-work tool steels. Die failure in Toyota's die-casting process also often occurs at around 10,000 shots. This record is considered a typical failure cycle, given the aforementioned evaluation cycle of hot-work tool steels and the exponential dependence of fatigue failure cycles. Consequently, this study assumes that the cracking phenomena targeted in these dies are predominantly classified as low-cycle fatigue, which is a type of fatigue fracture caused by thermal stress. Therefore, the maximum compressive strain was selected as the target for prediction.

The calculation of the maximum compressive strain employs the Adventure cluster, which is sold by SCSK Corporation. The governing physics equations for compressive strain are used in this calculation. The stress integration employs the Backward Euler integration metho [15], where the trial stress in the elastic predictor step is calculated and corrected onto the yield surface if it exceeds the yield stress (equation 4.1) Specifically, the trial stress $t'\sigma(T)$ is computed using the elastic constitutive tensor CCC, and if it exceeds the yield stress, it is corrected back to the yield surface using the plastic strain increment Δe^p to obtain the final stress $t'\sigma(F)$.

The equation used for this correction is:

$$t'\sigma_{(F)} = t'\sigma_{(T)} - \frac{3}{2}\frac{\Delta e^p}{t'\sigma_{(F)}}\, 2G\sigma'_{(F)} \qquad (4.1)$$

Where G represents the shear modulus of elasticity. The term $2G\sigma_F'$ ensures that the stress is corrected back to the yield surface if it exceeds the yield stress.

The numerical values obtained after the calculation are transferred to a voxel-based 3D model and linked with the shape feature quantities extracted by a 3D VAE (Variational Autoencoder), which are then used as training data for the machine learning model described later.

4.2 Parts to be Analyzed

This study analyzed 113 kinds of engine block parts and 130 trans axel cases produced by Toyota Motor Corporation by die casting in the past. Figure 2 shows an image of the product shape. In this study, detailed in Chapter 5, a surrogate model is constructed using voxel-based shape information. Consequently, the CAD model is converted into a voxel-based model composed of 1.6mm cubes. This model conversion is carried out using the post-processing functions of TopCAST, a casting analysis CAE software provided by TOYOTA SYSTEMS Corporation. Additionally, the analysis model used in the stress analysis on the Adventure cluster mentioned earlier is not voxel-based, making it impossible to link the shape and analysis values directly. To address this issue, the analysis model from the Adventure cluster is superimposed onto the voxel-based model, and the nearest simulation results are mapped to each voxel. This mapping is then utilized to construct the subsequent surrogate model. Table 1 summarizes the maximum, minimum, and average values of the shape and volume of the engine block, and Table 2 provides the same for the transaxle case.

Figure 2: Image of product shape (a)Engine block, (b)Trans axel case.

	width[mm]	length[mm]	hight[mm]	volume[mm^3]
max	252	417	242	8151175
min	184	410	239	7911446
average	217	412	240	8060845

Table 1: Engine block shape and volume statistics.

	width[mm]	length[mm]	hight[mm]	volume[mm^3]
max	474	649	253	4250977
min	175	491	134	3364684
average	361	534	173	3929535

Table 2: Trans axle case shape and volume statistics.

5 CREATION OF A SURROGATE MODEL

The procedure for constructing the surrogate model is as follows. First, for each voxel on the surface of the 3D model, which is entirely voxelized, a cube with a side length of 48 mm centered on the voxel is cut out. Then, a Variational Autoencoder (VAE) is trained using the cubic shape created at each point on the surface. Through this process, an encoder that can translate the cubic shape feature into a vector is obtained. Finally, a neural network is trained with the feature vector as input and the simulation result at the center of the cube as output. The flow of estimation is illustrated in Figure 3. In this study, 20 parts from each of the 113 parts of the engine blocks and 120 parts of the trans axel cases were used to train the VAE, and the remaining parts were used to train the NN. Further details regarding the VAE and neural network structure will be described in the following sections.

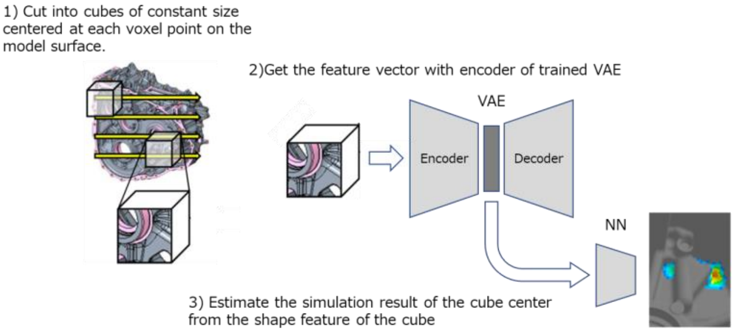

Figure 3: Image of constructing the surrogate model.

5.1 Evaluation Method of Surrogate Model

When the CAE analysis results and the predicted results from the surrogate model were plotted on the 3D model geometry, the clumps of regions with values above a threshold were each defined as soldering regions, and the degree to which the regions in the CAE analysis results and the regions in the predicted results matched over the entire part was evaluated. A program using Python was created to determine and compare the regions, automating the entire aggregation process.

In this study, the F1 score was used as the evaluation index, and the threshold value at which the F1 score is the maximum was obtained for both the surrogate model and the rule-based model.

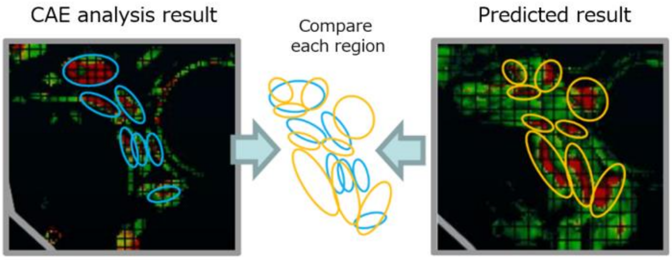

Figure 4: Image of evaluation method.

5.2 Voxel-Based Variational Autoencoder and Neural Network

The Variational Autoencoder (VAE) constructed in this study is inspired by models that have demonstrated high accuracy in object classification tasks. A VAE is a type of autoencoder, which is a neural network trained to reproduce input data at its output layer. The 'variational' part refers to making it a probabilistic graphical model by adding a stochastic layer. VAE compresses data into a lower-dimensional space and then reconstructs it back into the original space. During this process, the VAE learns to capture the intrinsic features of the data in this lower-dimensional space, generating feature vectors. The specific structure of the model follows one that has previously shown success in die-casting. Before finalizing the architecture, preliminary experiments were conducted to ensure the structure adopted would guarantee accuracy. The factors that significantly impacted accuracy included the input cube size, the type of activation function, and the weighting of the loss function. It is suggested that these aspects be referred to as proper parameter tuning, which may be required depending on the nature of the problem. After training the VAE, the feature vectors extracted from the latent space serve as inputs for another neural network designed for regression prediction. This neural network is a four-layer multilayer perceptron that includes dropout, consisting of an input layer with 100 nodes, two hidden layers with 50 and 10 nodes, and a single-node output layer. Following each hidden layer, there is a batch normalization layer with an epsilon of 2e-5 and a dropout layer with a dropout rate of 0.25. The activation function between layers is the leaky ReLU function with a negative slope of 0.2, and the output layer uses the soft plus function. Details of the learning process are described in Chapter 5.3, 'Model Training'.

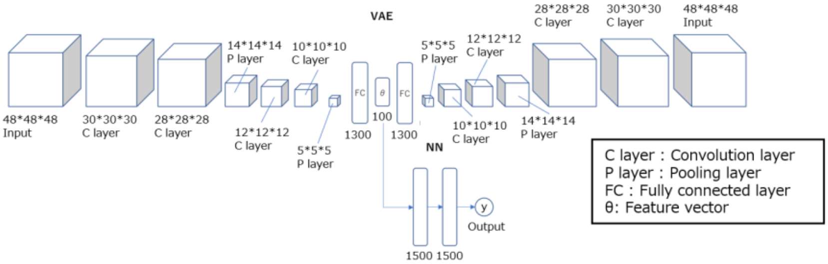

Figure 5: Architecture of VAE and neural network.

5.3 Model Training

For the VAE, the training was conducted with a batch size of 10 and for one epoch with a learning rate of 0.001. The optimizer used was AdaGrad, and the loss function parameters included a reconstruction error calculation sampling number of 1 and a KL divergence term coefficient of 1. For the Neural Network, the training was conducted with a batch size of 32 for one epoch and a learning rate of 0.001. These parameters ensured the appropriate progression of learning for each network. Figure 6 shows the training curve of (a) VAE, (b) Neural Network for Engine Block, and (c)Neural Network for Trans axel case. We can see that each of them was trained appropriately. The results confirm that learning progressed appropriately in each network.

6 EVALUATION RESULT

We evaluated the performance of models for predicting the occurrence of die cracks in both engine block parts and transaxle case parts. The performance of the models was assessed using the F1 score, which is the harmonic mean of precision and recall. For the engine block parts, there were 594 True Positives (TP), 208 False Negatives (FN), and 530 False Positives (FP), resulting in an F1 score of approximately 0.62. For the transaxle case model, there were 174 TPs, 73 FNs, and 178 FPs, with an F1 score of about 0.58.

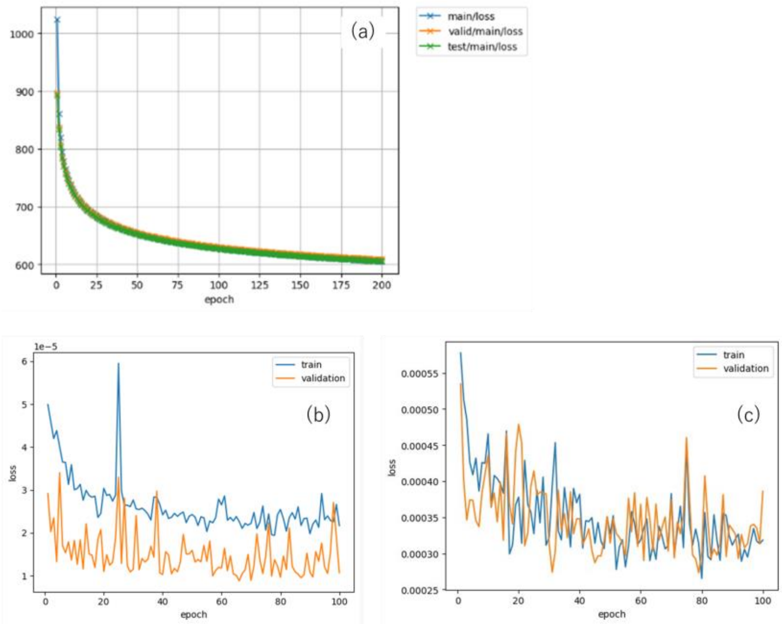

Figure 6: Train curve of a) VAE, b) Neural network for the engine block, and (c)Trans axel case.

Figure 7 illustrates the trend of the F1 score as the decision threshold was varied for both the engine block and transaxle case models using a line graph. The results indicate that it is possible to achieve a relatively high F1 score in both cases. Next, to assess how the performance compares to that of a previously implemented surrogate model for predicting die soldering [12], we tested the difference in precision between models using the bootstrap method [16]. When resampling bootstrap samples, we created sub-samples for each product shape and conducted tests for differences. Figure 8 shows the bootstrap distribution of differences as a histogram. The results suggest that the difference in F1 scores between the surrogate model for previously reported die soldering and the surrogate model for die cracking developed in this study does not reach the 90% confidence interval. Therefore, the approach in this endeavor is considered capable of achieving the same level of predictive accuracy for multiple types of defects in the die-casting process.

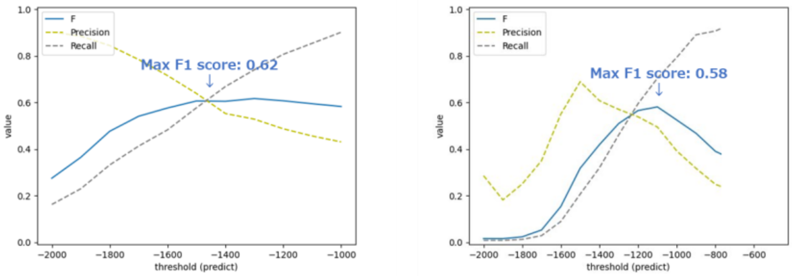

Figure 7: Transition of F1 score of a) Engine block's surrogate model and b) Trans axel case's surrogate model.

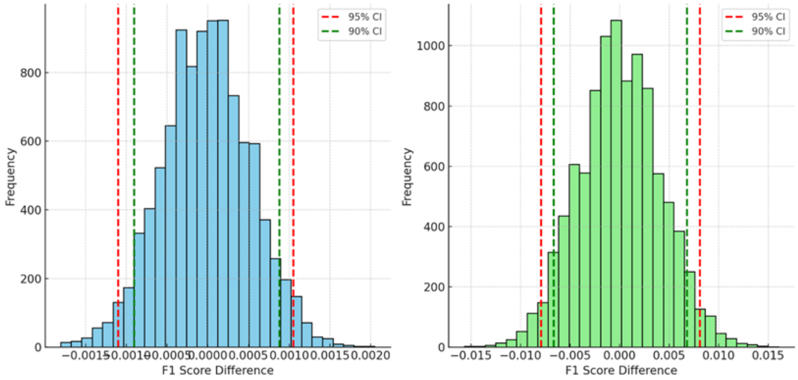

Figure 8: Bootstrap distribution of F1 score difference between (a) Engine model and referenced model, and (b)Trans axel case model and referenced model.

The accuracy shown in Figure 7 was obtained when all the data prepared for this study was used for training, but Figure 9 also shows the accuracy when the amount of data was small. As can be seen from Figure 9, the improvement in accuracy with the increase in data volume appears to be somewhat saturated. Therefore, in order to achieve further improvements in accuracy, it is likely that a fundamental change in the learning architecture, rather than an increase in data volume, will be necessary.

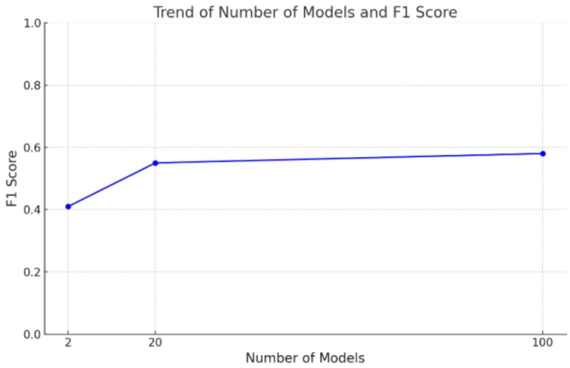

Figure 9: Trends of the Number of Engine block models and F1 score

7 CONSIDERATION OF PREDICTION ACCURACY

In this study, we constructed a surrogate model for predicting cracks in die-cast dies and achieved a certain level of accuracy. This model evaluates the risk of cracking based on the structural features of the die and conditions during the manufacturing process. However, the application results of this model showed many false positive cases where the predicted cracks did not actually occur. This suggests limitations in the model's predictive performance and indicates the need to investigate the causes and consider countermeasures.

Particularly noteworthy is the area predicted to crack in Figure 10, which has a deep valley-like shape. Such a shape seems reasonable to predict as having a higher risk of die cracking due to the stress concentration caused by the notch effect. However, a detailed investigation of the actual die cross-section, as shown in Figure 11, confirmed that it is sandwiched by cooling circuits on both sides. These cooling circuits may limit the occurrence of stress by suppressing the temperature rise during contact with molten metal and reducing the temperature gradient.

In addition to these design approaches that are not apparent in surface shape, efforts such as reducing the amount of release agent to prevent rapid cooling and manufacturing the die from high thermal conductivity materials to alleviate rapid temperature gradients are undertaken to mitigate thermal shock and thermal fatigue [17]. Furthermore, since the type of die material also affects fatigue strength, the timing of crack occurrence varies even with the same thermal shock. To address this, selecting materials with high fracture toughness and applying thermal treatments that enhance grain refinement can significantly improve the die's resistance to thermal fatigue. By refining the grain size through processes such as thermal cycling or controlled quenching, the material's ability to withstand cyclic thermal stresses without crack initiation is enhanced. This approach, based on recent advances in the understanding of the limits of strength and toughness in steel [18], ensures that the die maintains its structural integrity under extreme conditions, thereby extending its operational life and reliability.

Therefore, predicting the risk of cracking based solely on the surface shape of the die has limitations, and it is necessary to consider more detailed information, such as the internal structure, the arrangement of the cooling system, and other measures to prevent thermal shock and thermal fatigue. Such exceptional data could act as noise in the learning process of the surrogate model, potentially leading to a decrease in prediction accuracy. Future research should aim to accurately identify these exceptional cases and optimize the model's learning data. Moreover, incorporating more multifaceted factors into the model, such as the arrangement of cooling circuits and the temperature distribution within the die, is expected to reduce the occurrence of false positives and enable more reliable predictions.

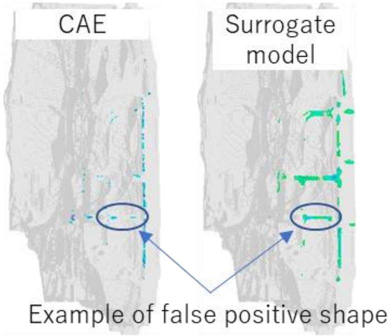

Figure 10: Example of (a) rule-based prediction and (b) actual die model.

8 CONCLUSIONS

The evaluation results suggest that it is possible to construct a surrogate model with a certain degree of accuracy using only product shape by leveraging VAE and NN for die-cast die crack prediction. However, when the product shape on the opposite side includes distinctive shape elements such as cooling circuits, the stress impact on the die from shape characteristics applied in this study cannot be fully accounted for, leading to decreased accuracy in these areas. Including detailed die design features in the learning data could improve accuracy, but the primary motivation of this endeavor was to predict defects from product shape alone, which may represent an inherent limitation of the approach used in this study.

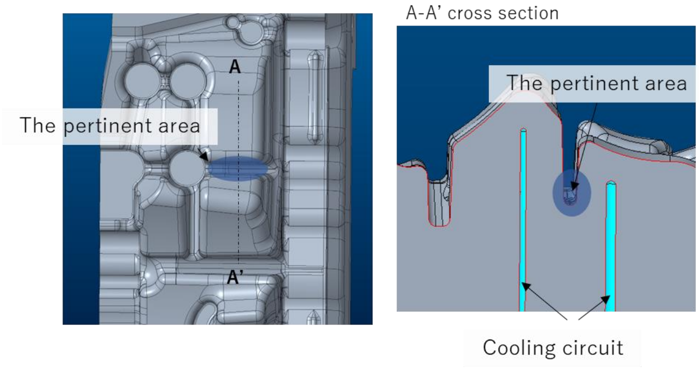

Figure 11: Die architecture of the pertinent part

Additionally, the data used in this study, whether for transaxle cases or engine blocks, required a large number of 3D models and simulation results. Collecting detailed product development-related data on this scale is generally challenging, which could limit the application of this approach in other contexts or smaller-scale projects.

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