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Probabilistic Property Modeling for reliable Casting Design and Production

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Keywords

Probabilistic modeling, casting process simulation, process variability, microstructure modeling, tensile properties, robust component design

Abstract

A new methodology leverages virtual casting process simulations to predict the statistical distribution of local mechanical properties, based on computed local microstructures and defects. The extensive result sets generated from each simulation can be statistically evaluated in a manner similar to numerous individual tensile tests. By incorporating process variability into the simulation, this innovative approach enables probabilistic modeling of expected local properties. Consequently, this method supports designers during the design phase for reliable component development and assists casters in achieving robust process designs.

Introduction

Casting process simulation has been utilized for 40 years to provide insight into the casting process, predict potential problem areas, and help experts optimize their casting design and engineering decisions. In addition to the growing capabilities of simulation software, the key to increasing the utilization is the delivery of quantitative information to the right people at the right time. Traditionally, information from casting process simulation has been successfully used downstream in the engineering of the casting process. At this stage, most of the cost-relevant decisions about component design and the selection of the casting process have already been made. The earlier the information is implemented in the design process, the more design freedoms are created and related cost savings can be realized.

Robustness of cast designs

In the design phase, the designer does not know the final process conditions, so they must design the component with uncertainty in mind. The relationship between defining the process , local microstructure, defects and final mechanical properties is considered using safety factors in the component design and specifications. Consequently, the potential of the alloy used is therefore not fully exploited, making the part unnecessarily heavy.

This is a typical "chicken or the egg" problem: How can I optimize the casting geometry for the material without having detailed knowledge of the manufacturing conditions at this stage? Often, the supplier has not even been selected at the time of the design freeze, meaning the window of opportunity to incorporate process simulation information is minimal. The designer must account for the uncertainties of undefined process constraints, leading to the use of safety factors and demanding specifications for the supplier. Consequently, casting customers demand certain quality levels from their suppliers and specific property levels for different areas of the casting (Figure 1), depending on the load case, which reduces risk. The supplier is responsible for the resulting production and quality costs.

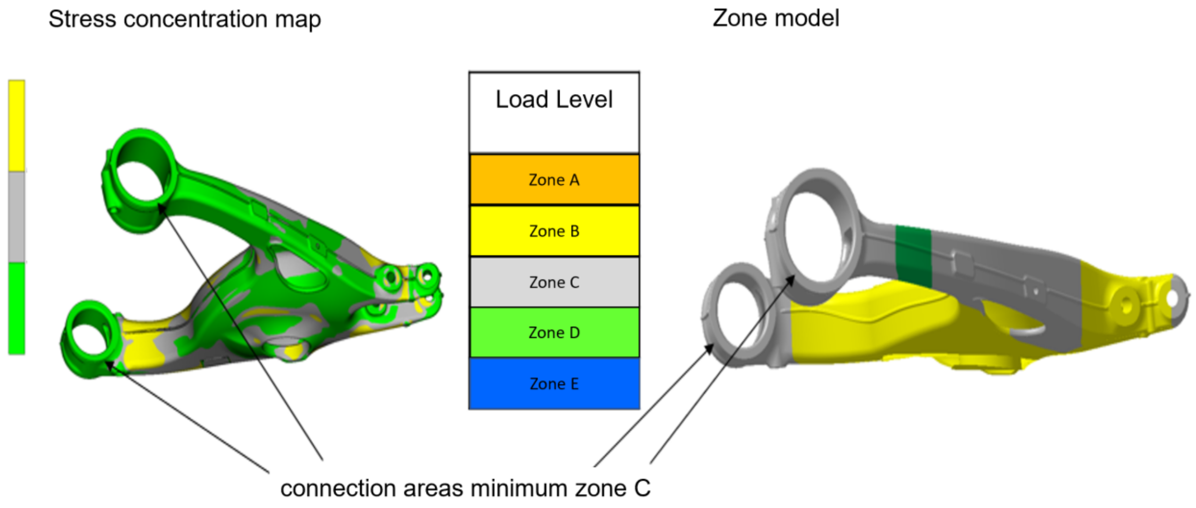

Figure 1:Technical Specification for Aluminum Sand, Gravity and Die Casting. Division of the component into zones of equal strength, left. A zone model is derived based on results from e.g., durability calculations, crash simulations and misuse cases. The zones tolerate different defect sizes and frequencies, right [1].

Robustness of the Casting Process

Once the component design has been completed, decisions must be made about casting technology, tooling and process windows. At this stage, other players, such as the toolmaker and casting facility get involved. Simultaneously, the number of parameters influencing part quality and associated mechanical properties increases significantly. To obtain a robust mold design and process condition, it is standard to use information from individual simulations or virtual trial planning with the help of casting process simulation. These analyses allow the determination of ideal operating conditions and the establishment of a robust process window for the expected mechanical properties of the part.

The toolmaker designs the gate and mold according to the required part quality, while the engineer in the casting facility sets operating conditions that ensure a smooth and short ramp-up phase. This information also allows the quality manager to inform his customer (i.e., the part designer) of the expected variation before the first part is produced. However, these activities come too late to optimize the casting design itself.

Simulation of Casting Properties

Casting process simulation has been used for 40 years to identify potential casting defects at an early stage and avoid them by optimizing the casting technique [2]. In the early 1990s, models were developed that could provide information on the expected local microstructure in addition to macroscopic predictions of flow, heat flow, and stresses. These so-called micromodels use theories of nucleation, crystal growth kinetics and segregation behavior of the melt, coupling them with the macroscopic heat flow to calculate local microstructures [3]. The knowledge of the local proportions and the formation of different phases also made it possible for the first time to predict local mechanical properties (Figure 2).

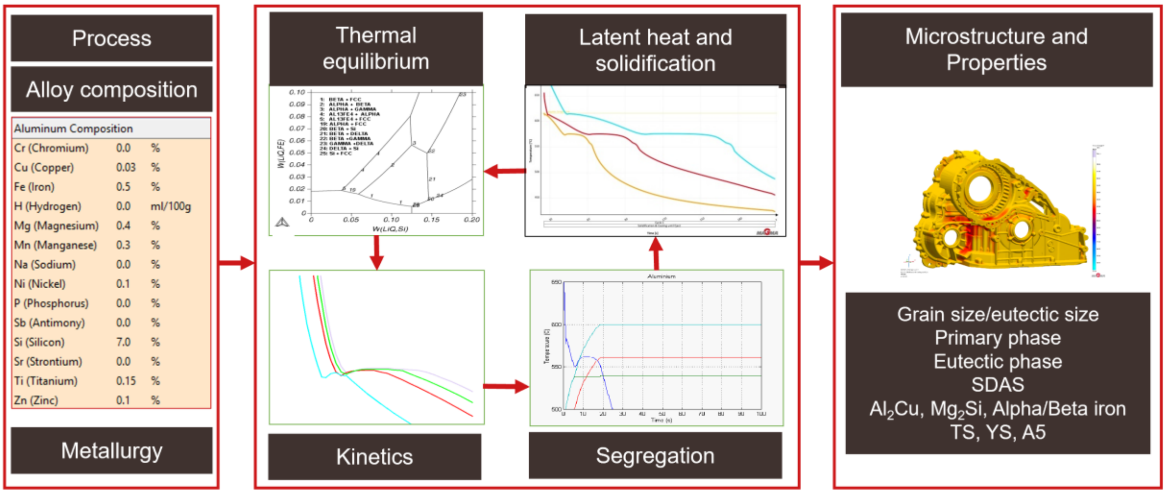

Figure 2: Principle of microstructure simulation of aluminum materials. In addition to the classical input variables for the process, the alloy composition and the metallurgical state of the melt can be taken into account and influence the results.

The advantages of using micromodels over purely macroscopic calculations lie in the additional information they provide on local microstructures and properties. Microstructure simulation allows for variation in alloy composition as an input parameter and can account for different metallurgical and inoculation states. This method is useful for predicting properties whenever the basic microstructure significantly influences local mechanical properties. This is especially true for cast iron materials and controlled casting processes in light metal casting. Consequently, these models have been adopted early on for these material groups and processes [4-7].

In casting processes where material failure is predominantly determined by imperfections in the casting, predicting local mechanical properties based solely on the calculated microstructure can be problematic. This is particularly true for high pressure die casting, where the local properties are determined by the turbulent mold filling, which occurs in milliseconds, and the rapid solidification, both of which introduce various defect mechanisms. Significant defects that lead to natural weakening of the microstructure include shrinkage-related pores, gas porosity from air inclusions and hydrogen precipitation, as well as oxides, cold runs and microcracks (Fig. 3). The individual modeling of these defects in casting process simulation has also made significant progress in the last 20 years.

Most of these defects, especially oxides and inclusions, occur discreetly and stochastically distributed in the casting, even with a robust process condition. Therefore, distributions and fluctuations can only be quantitatively predicted to a limited extent by the deterministic models described above.

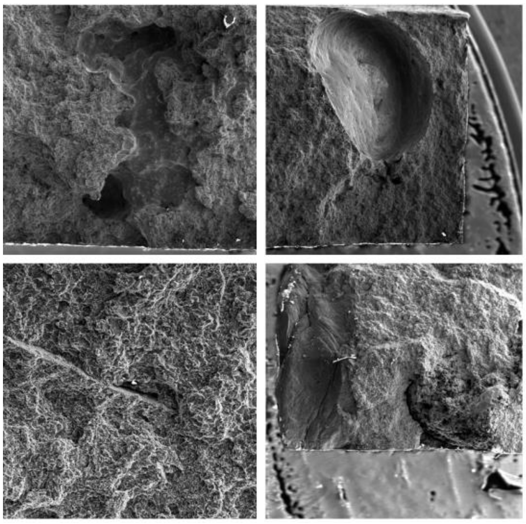

Figure 3: Typical casting defects in die casting: microporosity (top left), entrapped air and hydrogen precipitation during solidification (top right), oxides (bottom left), or cold running (bottom right).

To make reliable predictions about the expected local properties for the high pressure die casting process, the methodology of "quality mapping" was developed in the early 2000's. Here, extensive measurements of mechanical properties in the component were correlated with existing quality criteria from the casting process simulation and used to predict the local component behavior [8-11]. The advantage of quality mapping is that it validates stochastic fluctuations in casting quality through real test planning. However, a disadvantage is that the determined correlations cannot be arbitrarily transferred to other components or processes (Figure 4).

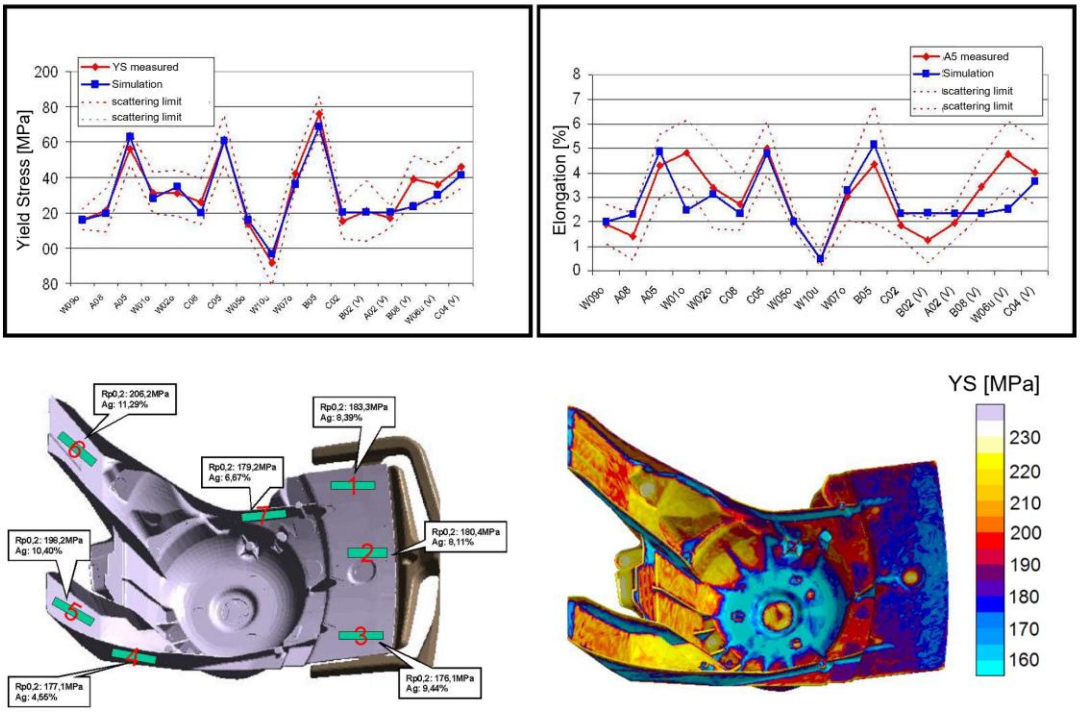

Figure 4: Property prediction by quality mapping for a die-cast strut dome. Correlation of a) yield strength and b) elongation at break with tensile test results [9].

The predicted local material properties, including the effects of local defects, can be transferred to FE-analysis of the part subjected to static, fatigue, or thermo-mechanical loading [12-16]. Component designers have long used these capabilities in component design CAE programs to investigate the influence of varying casting properties on loading [17]. The first applications included accounting for residual stresses resulting from heat treatment of cylinder heads [18-20]. Simulated information on local properties can also be used in fatigue analysis [21, 22] (Figure 5). However, this is only accepted in practice if the minimum expected local properties are statistically validated.

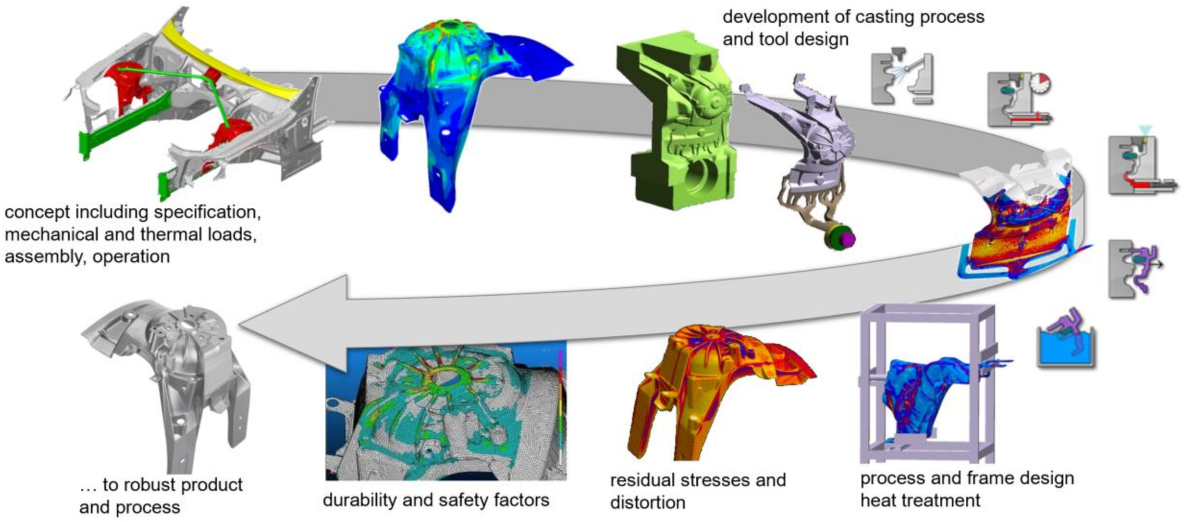

Figure 5: Integrating casting process simulation results into product development and process design.

From Deterministic to Probabilistic Modeling

Most people have a deterministic mindset. This is what we were taught in school: input certain values into an equation and you will always get the same result. This way of thinking is often applied to material properties (e.g., by using values from standards as fixed values in calculations). People tend to think that we are moving away from physics (or accuracy) when we start using statistics. The assumption is that if I keep my process constant, everything should stay the same.

The use of deterministic models in casting process simulation has significant strengths. If the model allows prediction of a property or defect, then any change in the input parameters -such as part design, die design, casting technology, metallurgy, alloy composition, and process parameters- leads to a measurable response in the results. The implicit strong coupling between "input" and "output" makes it possible to achieve the desired objective (quality, productivity or cost) by systematically changing the input parameters. However, this is where the model differs from reality, as the coupling of process data to part quality is very weak due to the time factor and the incomplete and often indirect measurability of both the input variables and the casting quality.

Since the 2010’s, the implementation of virtual test planning and automatic optimization in simulation has created opportunities to complement the usual sequential approach (determination of casting conditions, simulation, evaluation of results for a next variant). This allows for a holistic investigation of production windows and the determination of optimal conditions for the respective objective [24-27]. It also enables a systematic investigation of production variations by varying the process conditions with different simulations (Figure 6).

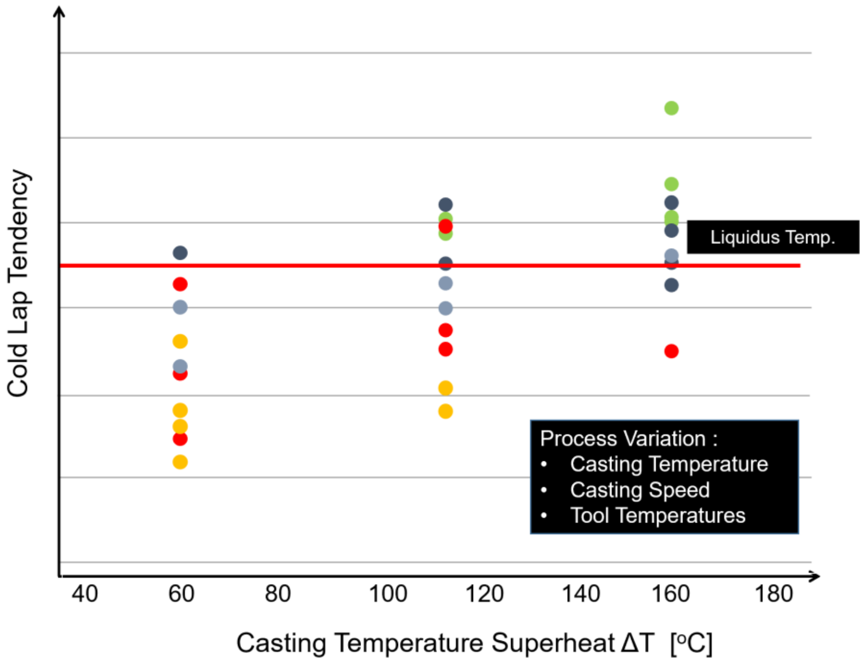

Figure 5: Systematic investigation of process variations on the tendency of cold runs with casting process simulation using a virtual test plan. Each point corresponds to the result of a simulation with different process or boundary conditions. The evaluation criterion is the liquidus temperature. In this example, the process variations investigated (casting temperature, shot time, and mold temperatures) lead to cold runs in only two out of ten variants when the melt overheats by 160 C. At 110 C, seven out of ten variants are at risk of being rejected, and at 60 C, nine out of ten variants are at risk of being rejected.

The weakness of the deterministic approach remains that in a single simulation, the simulated defects or properties vary locally but have no dispersion. This is a fundamental problem when evaluating a simulated defect.

Confidence in the predictive quality of casting process simulation is often so high today that the predicted defect is accepted as "real". However, a single simulation represents just one virtual attempt. Simulating the same scenario ten times will yield the same result each time, whereas reality in the foundry involves accepting production variations and the consequent changes in quality. Foundry production staff aim for a process window that is as robust as possible to absorb natural variation.

When foundry staff discuss scrap, they typically refer to percentages like 5% or 2%. This means that only every 20th or 50th part exhibits the defect predicted by the simulation. In addition, depending on the specification, a real defect may be classified as such or even neglected (Figure 7):

- For instance, if the allowable pore size is 1 mm, what about 0.9 mm?

- Similarly, if the acceptable defect zone has 4 pores within a 25 mm^2 area, what if there are 6 smaller pores totaling the same area?

Furthermore, depending on the location or minor local variation, the identical defect may either be deemed acceptable or cause the part to be scrapped, despite the simulation results remaining unchanged (Figure 8).

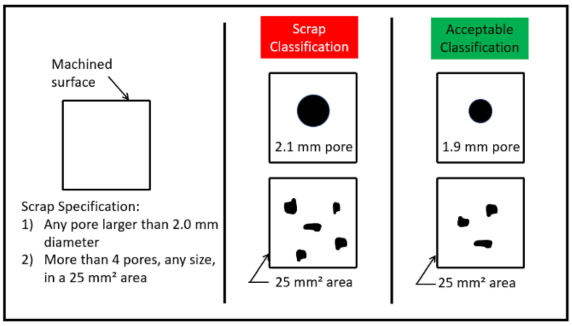

Figure 6: Specification of reasons for rejections in the casting. The smallest fluctuations in the measured error variables can lead to rejects, depending on the limit value [28].

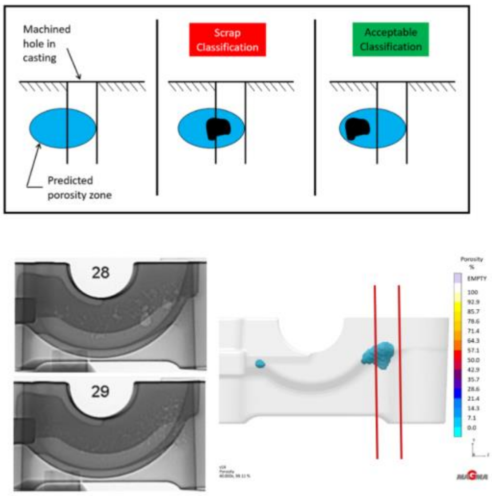

Figure 7: Comparison of simulation results with real failure patterns. The simulation shows a region where defects occur. However, depending on the location and specification, the real defect is critical or acceptable [28].

There is often a misconception that if deviations exist between reality and simulation, the calculated results are inherently "wrong". Unlike many properties that vary continuously, defects such as pores are singularities with discrete values —they are either present or absent, and within the acceptable or critical range. However, when the real distribution of measured scatter overlays the deviation between simulation results and actual measurements, simulated errors predominantly align with the normal distribution of real fluctuations (Figure. 9).

As mentioned, instances of erroneously rejected results are more likely outliers than the norm. Therefore, each simulation result should be viewed as representing the maximum probability of defect occurrence, rather than as a precise geometric characteristic.

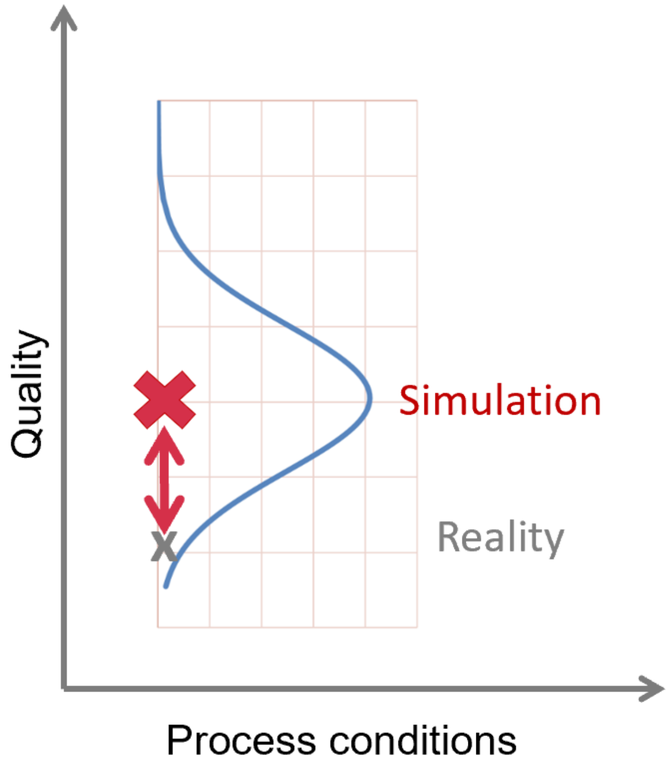

Figure 8: Deviation between simulation and reality. Apparent discrepancies between the results of a simulation and an observed defect can often be explained by different probabilities.

Probabilistic modeling of mechanical properties

The molten aluminum entering the mold will not only contain atoms of the specified chemical composition, but it will also invariably include a stochastic distribution of oxides and other inclusions. The extent of potential damage to the material depends on the amount of these defects already present in the melt when it is poured into the casting chamber (which we can never precisely know in the simulation or specify as a fixed boundary condition). It also depends on how much is generated during mold filling and solidification (which we can better predict). Therefore, there is a physical rationale for introducing a "process variability" parameter into the simulation, which describes, for example, the "degree of damage" to the melt even before the simulation begins. This factor is highly dependent on the quality of the raw material and the melt treatment in the foundry prior to casting.

Mechanical properties in castings not only follow the nature of the underlying physical phenomena, but also adhere to stochastic principles in terms of material deformation and failure. The elongation of the material up to failure must therefore be understood as a problem of the “weakest link”. Oxides play a significant role here due to their shape and size and inclusions due to the high local stress concentration (Fig. 10) [29]. The scatter of these failures causes naturally follows a stochastic distribution rather than just a deterministic value (Fig. 11) [30,31]. Combining the deterministic models of casting process simulation with a probabilistic approach thus provides a method that better represents the underlying physical phenomena.

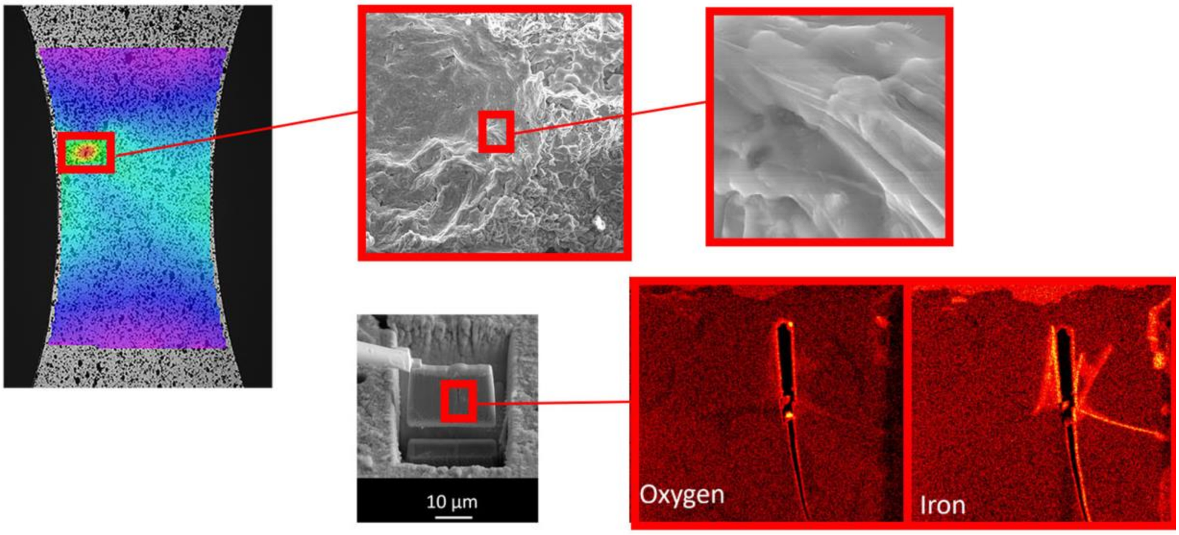

Figure 9: Determining the root cause of failure in a tensile specimen. Digital image correlation and scanning electron microscope observations of aluminum castings show that fracture is caused by an oxide layer that acts as a strain concentration under load [29]

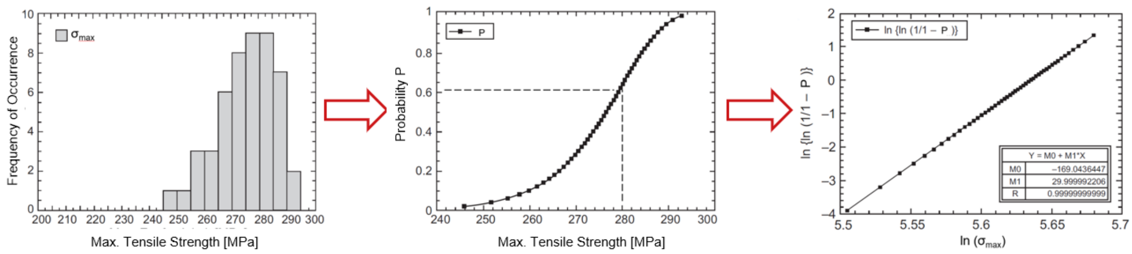

Figure 11: The real or calculated frequency distribution for the maximum tensile strength (left) can be represented as probability P (center). A Weibull analysis can be used to determine both the consistency of the data (straight line) and the minimum expected properties (right) [30].

If this behavior is accepted, the possibilities in the real world are very limited:

- How many specimens are needed to determine robust values for mechanical properties in a casting?
- How often must the test be repeated in a reproducible and reliable manner to obtain statistically valid data on material-related component behavior?
- Where can specimens be taken from the casting?

For reliable interpretation of material properties, averaging a few samples is not sufficient to provide statistically significant information about nominal values, much less to evaluate extremes or outliers.

Methodology for Probabilistic Modeling of Mechanical Properties

In a MAGMASOFT® simulation, the casting is often discretized with more than one million elements [2]. This means that for each calculated criterion, defect or property, a corresponding amount of information is available. These one million calculated values of mechanical properties can be interpreted as equivalent to one million tensile tests. Thus, it is reasonable to describe this as "big data," which is ideally suited for statistical evaluation. This approach allows the problem of error distributions and fluctuations, as described above, to be addressed probabilistically.

The methodology can be illustrated using a stochastic error distribution in a cast tension rod. Each calculated cell in the tie rod provides a different value for the expected microstructure, the calculated defects, and the resulting mechanical properties, Figure 12. The local ideal stress-strain curve for the material results from the microstructure simulation. The evaluation of the defects results in a statistical distribution that can be represented as a probability density function. This not only shows the strains at which the tension sample will most often fail, but more importantly, it indicates the statistical lower limit, i.e., the minimum strains to be expected. "This information can be mathematically described and exported as a field to other calculation programs with just a few parameters."

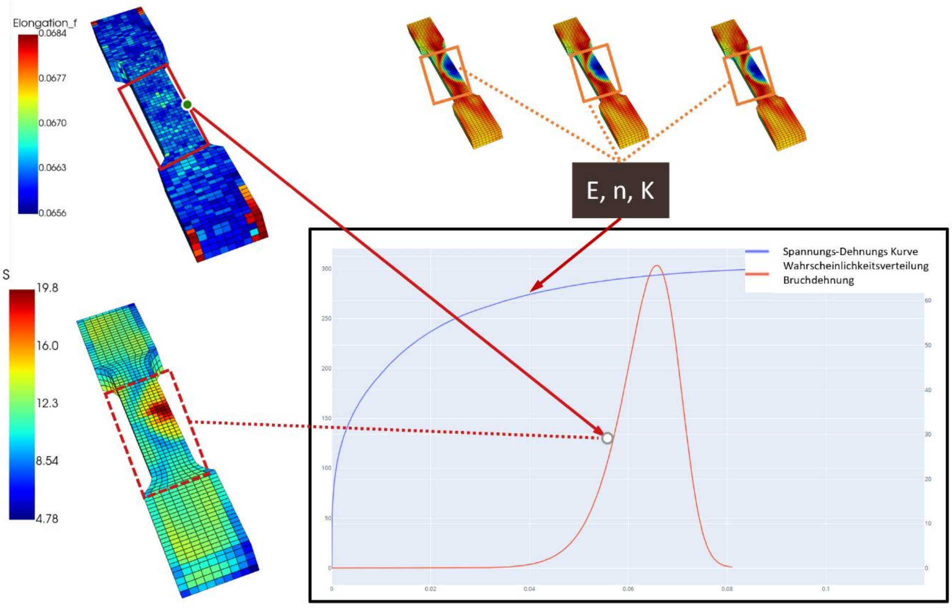

Figure 10: Distribution of calculated fracture strains A5 (top left) and their probability density function in a tensile member (bottom left). This information can be represented in a stress-strain curve and a probability density function and made available to other calculation programs with a few parameters (E, n, K).

The new methodology described below employs these concepts for probabilistic modeling of the mechanical properties of castings, as shown in Figure 13, using predictions from MAGMASOFT® in conjunction with the microstructure simulation for aluminum to locally calculate the mechanical properties of the microstructure and combines this with a statistical evaluation of the error distribution.

The following innovations are used.

1. Inclusion of an expectation function for process variability in the simulation.
2. Calculation of local stress-strain curves for the local microstructure using microstructure simulation.
3. Statistical evaluation of simulated defect distributions over a defined area and use of these static results as discount factors on the respective stress-strain curve at each location.
4. Statistical evaluation of the determined stress-strain curves for any area or zone with special load case or quality requirements, including the determination of distribution functions and minimum expected properties for each domain.

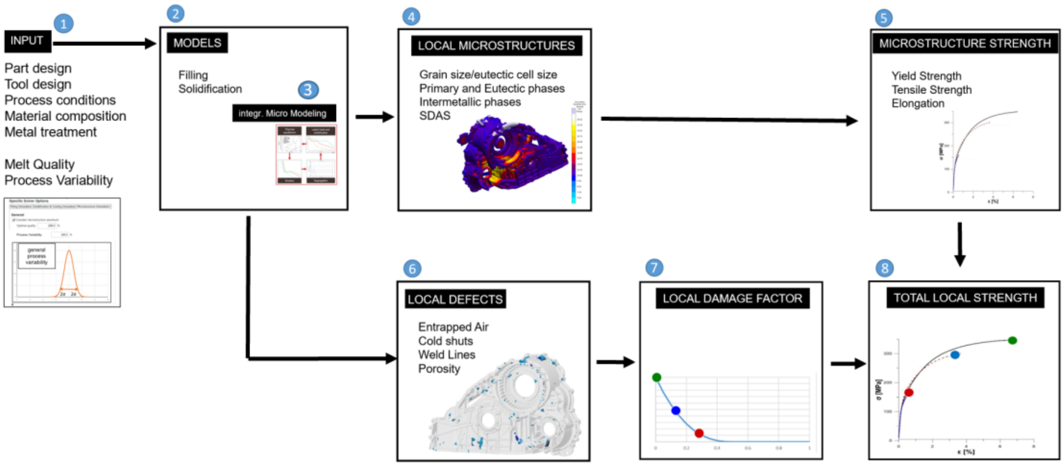

Figure 11: Flow chart of the core process of the methodology for a calculated design.

The methodology built into the software is as follows:

The user first defines the known status of the part geometry, tool design and process conditions for the current development status, along with the usual inputs for microstructure simulation, such as alloy composition and expected metallurgy. This constitutes the standard input information for any simulation (1). Additionally, a distribution function for the expected process variability is specified, which can be determined from practical experience from previous or similar projects.

This information is used to perform a single process simulation, which should be as detailed as currently possible, depending on the state of knowledge (2). The integrated microstructure simulation (3) is used to calculate local microstructure distributions for the material in addition to the classical, known results (4). These distributions serve as the basis for determining the local mechanical properties and the corresponding ideal stress-strain curves for each calculated microstructure (5).

At the same time, the software calculates the various errors to be expected for the entire component (6). For die castings, this is especially true for shrinkage porosity distributions and air inclusions. However, any other calculated criterion (e.g., for oxide distribution, cold run or cracking tendency) can also be used. A statistical evaluation can be performed for each of these defect criteria over a large number of cells to avoid the problem of deviations from discrete values. The mean value of the defect distribution is linked to the previously calculated local stress-strain curves for the respective area using a discount function, which can vary for each defect criterion (7). For each individual curve, this leads to a reduction of the ideal curve to the expected defect value (8) and thus to the expected distribution of the total strength in each calculated cell, Figure 14 (a). With the previously defined process variability, a stress-strain curve with a corresponding probability distribution is now available for each calculated cell in the casting, Figure 14(b).

This information can now be used in the software to perform further classical statistics on the distribution of properties in the casting. The user can decide which areas of the casting or which data sets to use for the evaluation. The software automatically determines the distribution of all calculated properties and their probabilities for predefined evaluation areas in the component. This can be understood as an extremely large number of tensile tests from the component, each supported by a virtual test scatter; Figure 14 (b).

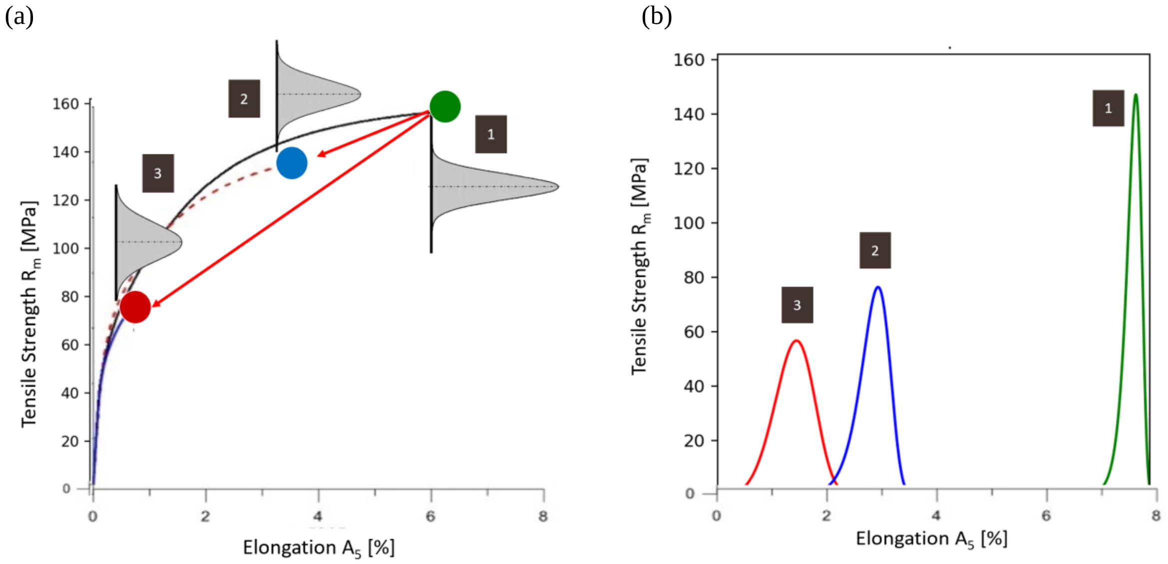

Figure 14: Calculation of total strength based on the determined defect distribution for three different locations in the part (a). Using the specified process variability, a probability function for the expected mechanical properties can be determined for each location in the casting (b).

This also allows Weibull analyses to be performed, showing distribution functions and expected values for the minimum expected properties in the respective range for the defined zones. The output is a series of expected minimum mechanical properties and the expected distribution for each evaluation range and their scatter (yield strength $Rp_{0.2}$, tensile strength R_m, elongation A_5), as illustrated in Figures 20 and 21 in the following chapter.

Applying the Methodology in the Development Process

Use Case: "Determination of Design Capability"

The methodology is applied with MAGMASOFT® on a die-cast transmission housing. To meet the requirements of the small-time window in the development process for determining „design capability", a process simulation is performed for a single design. Depending on the complexity of the part, this can be done in just a few hours.

After the usual definition of casting technology, tool and process conditions (Figure 15), the casting is additionally and automatically divided into so-called evaluation areas (EA) for the statistical evaluation of the calculated defects (Figure 16).

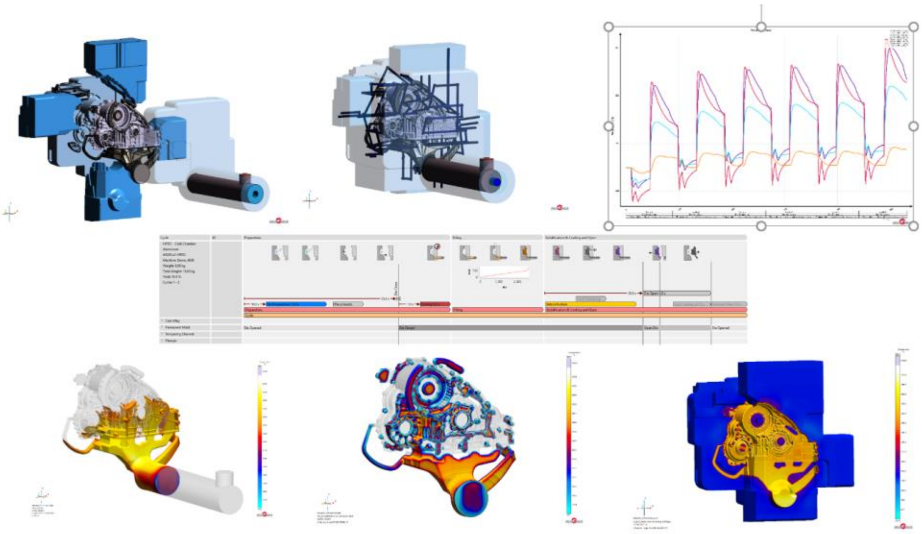

Figure 15: Process set-up and classic results of die casting process simulation: mold filling (bottom left), solidification (bottom center) and mold temperatures (bottom right) are the basis for probabilistic modeling of microstructures and properties.

The size of the evaluation areas and the corresponding number of cells can be freely defined by the user. Typically, several thousand cells are available in each evaluation area for the statistical evaluation of the calculated defects. For the output of the expected mechanical properties and their distributions, the casting is further divided into the specified zones of different requirements (Figure 16).

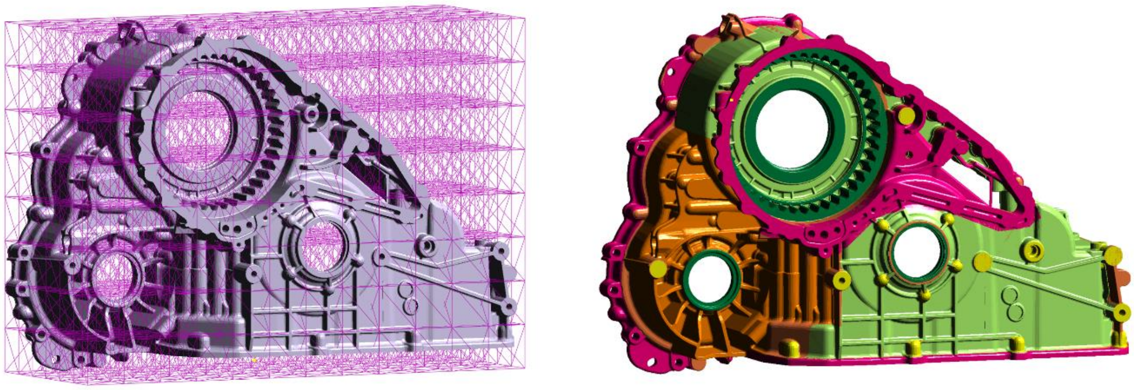

Figure 16: Partitioning of the casting into evaluation areas where the calculated defects are statically evaluated (left) and into zones with the same requirements specified by the designer (right).

The process simulation largely follows the familiar procedure. Additional information includes the definition of the alloy composition and the metallurgical parameters for inoculation and refinement used by the integrated microstructure simulation. Additionally, the newly introduced probabilistic parameter for process variability is defined.

Primary results from cycle calculation, mold filling and solidification represent well-known criteria, Figure 15. Additionally, microstructure and phase distributions along with intermetallic phases are calculated from the integrated microstructure simulation, Figure 17. This information is then utilized to derive the local ideal stress-strain curves, Figure 18.

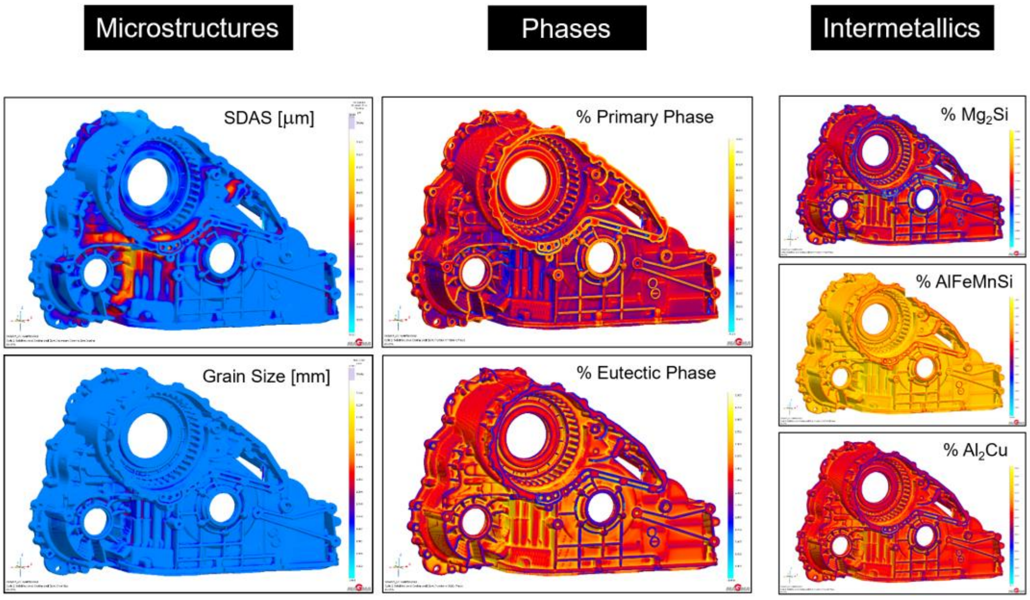

Figure 17: Results of the microstructure simulation. In addition to the quantitative distributions of microstructural features, phase proportions and the amount of (partially deleterious) intermetallic phases are also calculated.

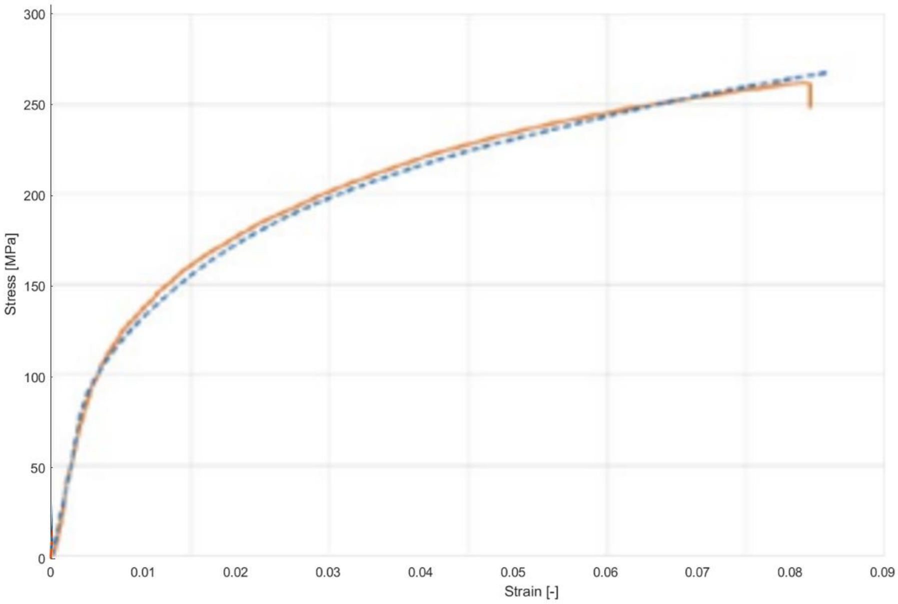

Figure 18: Comparison of the calculated ideal stress-strain curve of the matrix from the microstructure simulation with real measurements at a point in the casting.

The defect distributions simultaneously calculated in the casting (illustrated here for entrapped air and shrinkage porosity) are statistically evaluated in the defined evaluation areas, Figure 19. The damage value determined with the respective reduction factor is applied to the ideal stress-strain curves in each cell, thereby reducing the local tensile strength and elongation accordingly. Consequently, property distributions for yield strength, tensile strength and elongation at fracture are obtained, Figure 20.

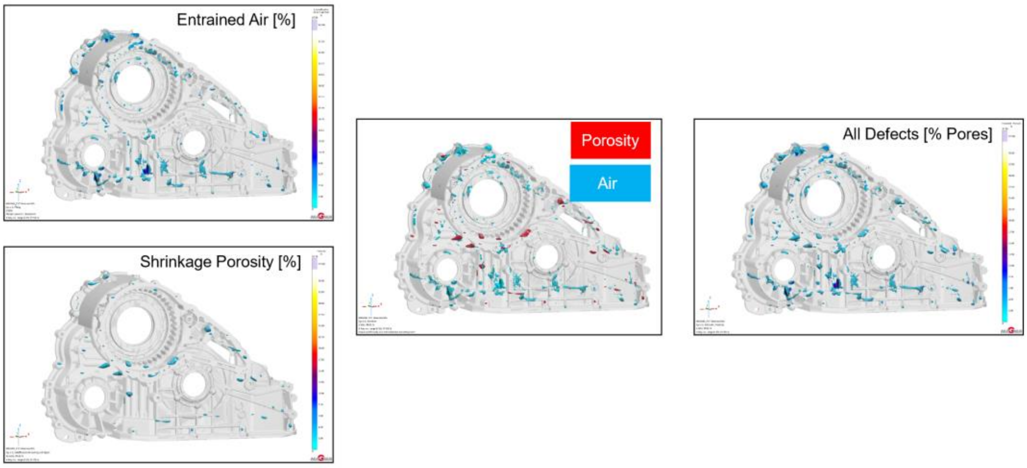

Figure 19: Evaluation of different defects for the gear case, here porosity and air inclusions

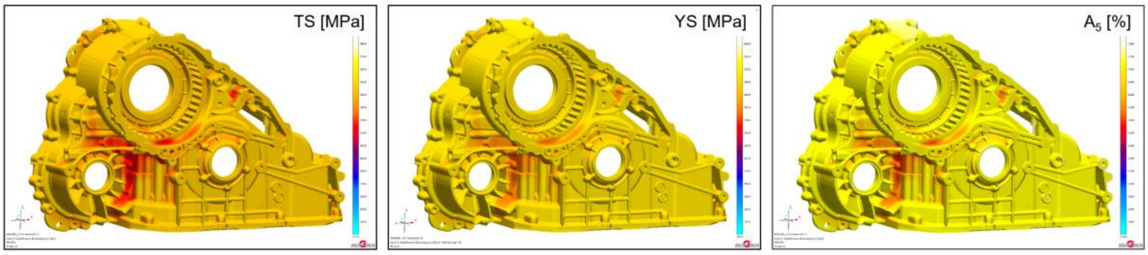

Figure 20: Strength distributions in the casting calculated using the methodology.

The data from all cells are statistically evaluated in a Weibull analysis for the evaluation in the defined zones. This allows a quantitative evaluation of the "Design Capability" of the component, Figure 21. An overview of the property distributions in the individual zones and the corresponding stress-strain curves determined for each zone, along with their probability density distributions, is presented in Figure 22.

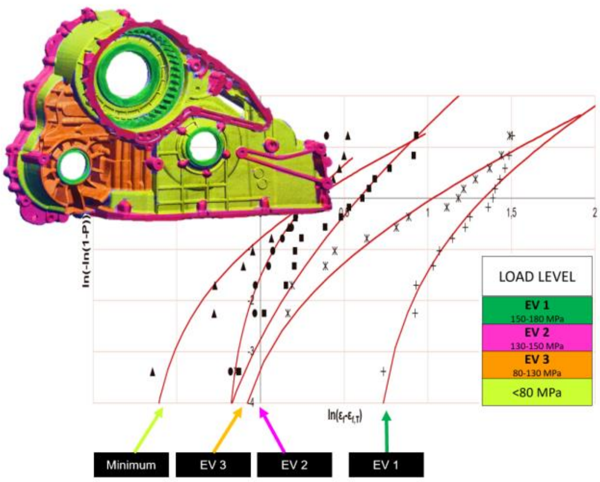

Figure 21: Statistical evaluation of the properties in different zones using a Weibull analysis of the calculated values. The curves demonstrate that the results align with statistically expected distributions. Additionally, the minimum expected properties in each zone can be inferred from the results.

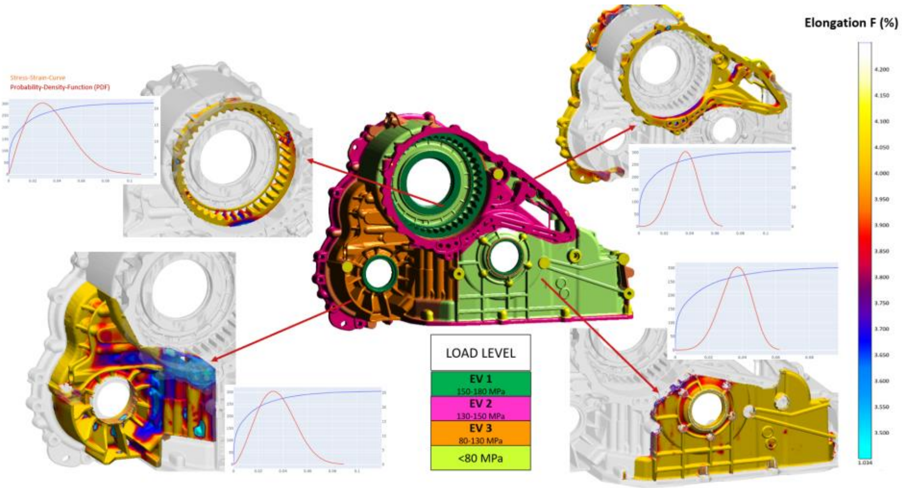

Figure 22: The methodology is applied to different zones within the casting, each with unique requirements. The curves illustrate the expected stress-strain curve and the distributions of mechanical properties at the statistical mean of each zone.

Use case "Determination of process capability”

In a later phase of the gearbox product development process, the casting facility that receives the order must design the casting process in detail. The die casters main objective is to use a casting and gating layout and process conditions that result in robust manufacturing conditions. This should create a process window capable of handling inevitable process variations at an acceptable cost. As no casting is defect-free, controlling defects and their impact on the specified quality levels (in the final mechanical properties) is of paramount importance.

The methodology used (Figure 23) is basically the same as in the evaluation of the design capability of the casting design (2)-(8). Instead of defining and running a process simulation for a single operating point (as in (1)), the die caster now varies the part and mold design (e.g., different gating concepts or cooling layouts) and the process window with several input variables (e.g., varied filling conditions such as slow shot, fast shot and switch-over point). It can also account for process variations (e.g., effects of operational interruptions on part quality) to define the input data for the DoE (11). Depending on the number of input parameters to be varied, several process simulations are performed automatically and without human interaction (12) to examine an entire process window.

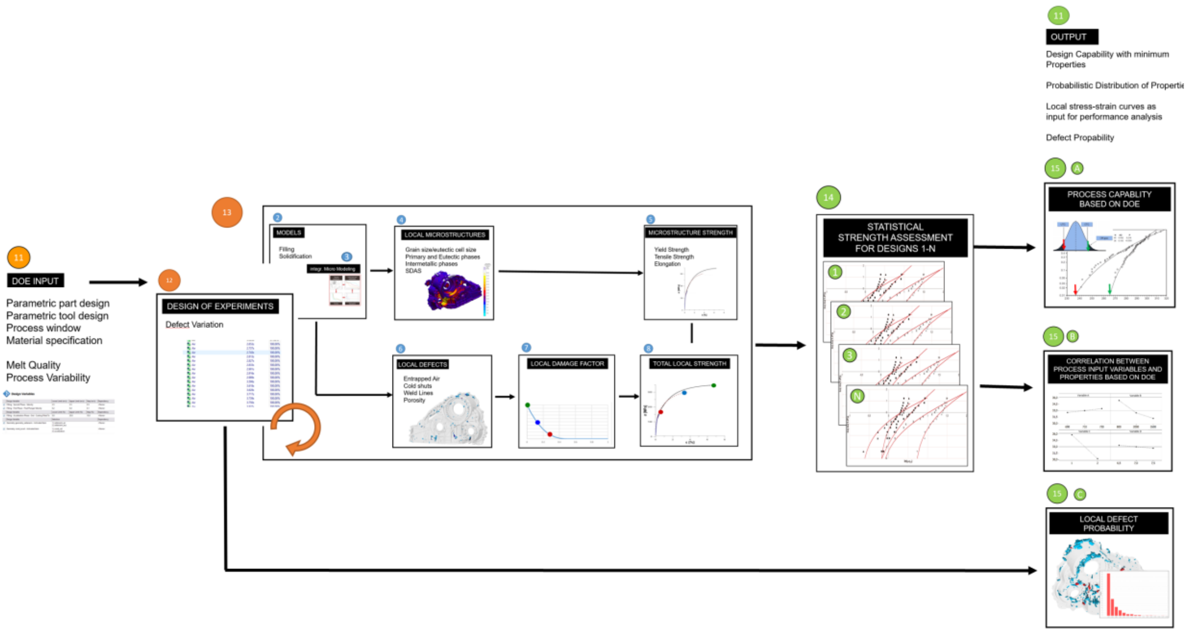

Figure 23: Flow chart of the overall process for determining process capability. Instead of a single simulation, the methodology is supplemented by a virtual test plan in MAGMASOFT®, in which all process parameters are systematically examined and evaluated.

The statistical evaluation (13 A, B and C) is similar to that previously described for the "Design Capability" use case. By varying the process conditions, the investigated process window and its process capability can now also be evaluated in relation to the expected properties. The evaluation tools integrated in MAGMASOFT® also allow the investigation of individual process variables with respect to the expected properties and the statistical investigation of errors in the process window, Fig. 24.

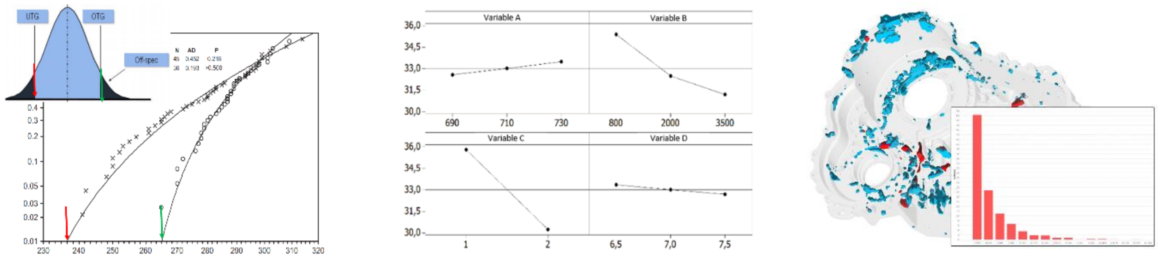

Figure 24: Key additional results of the process capability methodology: Expected process capability based on the examined virtual test plan (right); various correlations between process variables and expected properties (center); distribution of calculated defects in the casting (left).

Discussion

The presented possibilities for probabilistic modeling of properties, in combination with the deterministic models of process simulation, offer completely new approaches for validating cast part designs and selected process conditions. The results align to the reality of the process, where many variables can be accurately predicted, but process-related fluctuations that are difficult to model must also be managed. This is especially true for the stochastic error distribution resulting from metallurgy, melt treatment, and the casting process itself.

The integration of stochastics into the casting process simulation also has the advantage of separately and integrally considering differently calculated errors and their influence on the properties in the casting. Property distributions and minimum expected values can be evaluated over the entire casting, including any specific areas or zones. This is particularly beneficial for designing innovative new castings, especially structural components, where there is limited experience and high production and cost risks (hic: Giga Castings).

Due to the fast computation times for an individual simulation, results in information that can be used early in the development process for new castings. The workload for the user remains unchanged due to the automation of calculations and evaluation in the software.

When designing the die and process conditions, combining virtual test plans offers a systematic way to optimize the casting technology or process window. This approach not only focuses on error prevention but also investigates the influence on the required properties. The concept of performing numerous virtual tensile tests through simulation allows for the statistical evaluation of large amounts of data. This is a decisive advantage over real tests, which must be repeated many times to ensure reliable results.

Of course, the new method has its limitations. The quality of the results and their evaluation depends on the knowledge and accuracy of the defined input values for the simulated process. The better the models are at predicting the defects in the casting that specifically cause failure, the more accurate the statements about the expected properties will be. Additionally, the use of stochastics increases the reliability of the results and their application to component design and process control.

Summary and Outlook

40 years after the introduction of casting process simulation, combining the known capabilities of deterministic models with probabilistic methods marks a significant innovation for the predictive capability of casting designs and processes. The new patent-pending methodology presented here is not limited to die casting. It can be applied, with adaptations, to all casting processes and materials [33,34]. The methodology is still under development and requires further testing, particularly in real-world applications. Several industrial projects are currently underway with users, both OEMs and foundries [35].

Today, everyone is talking about the use of "big data" and the application of AI to determine correlations in order to control processes. In the foundry industry, identifying and managing large amounts of data is particularly challenging. This is due to the long development chain and the numerous factors influencing decisions. Many variables can only be measured indirectly and cannot be controlled, and a large number of factors that influence quality. Data can essentially only be determined during production, in which by that time all cost-related decisions have already been made. Casting process simulation does not have these limitations. Essential information and data can be generated at the design stage and before production begins. This provides an opportunity to apply AI concepts using data from the digital twin of real measurements. Probabilistic modeling also aligns with the foundryman's experience, which considers process variability, scrap rates, and property scatter. This methodology therefore offers the potential to significantly improve the acceptance of simulation results when using currently available models.

The methodology presented here enables addressing these challenges in virtual space, contributing to reliable component design and robust process control. The goal is not to predict the location of each pore 100% of the time. Instead, the aim is to provide the user confidence in the probability with which they can safely design or manufacture their casting.

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