On the use of heterogeneous thermomechanical and thermophysical material properties in finite element analyses of cast components

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Abstract. Cast components generally show a heterogeneous distribution of material properties, caused by variations in the microstructure that forms during solidification. Variations caused by the casting process are not commonly considered in structural analyses, which might result in manufacturing of sub-optimised components with unexpected in-use behaviour. In this paper, we present a methodology which can be used to consider both thermomechanical and thermophysical variations using finite element analyses in cast components. The methodology is based on process simulations including microstructure modelling and correlations between microstructural features and material properties. Local material data are generated from the process simulation results, which are integrated into subsequent structural analyses. In order to demonstrate the methodology, it is applied to a cast iron cylinder head. The heterogeneous distribution of material properties in this component is investigated using experimental methods, demonstrating local variations in both mechanical and physical behaviour. In addition, the strength-differential effect on tensile and compressive behaviour of cast iron is considered in the modelling. The integrated simulation methodology presented in this work is relevant to both design engineers, production engineers as well as material scientists, in order to study and better understand how local variations in microstructure might influence the performance and behaviour of cast components under in-use conditions.

1. Introduction
Numerical methods such as Finite Element Analyses (FEA) and topology optimization are commonly used by engineers in order to design and optimize cast components towards high load bearing capacity while simultaneously minimizing weight. However, if the analyst does not also consider the influence of the manufacturing process, the resulting component may become sub-optimised, or show unexpected in-use behaviour.

One important and often overlooked aspect is the spatially varying material behaviour in cast components caused by microstructural variations throughout the geometry. During the solidification of pearlitic hypo-eutectic flake graphite cast iron, a dendritic austenite structure grows as the primary phase, with features governed by the chemical composition and the inoculation conditions [1]. Graphite is precipitated together with eutectic austenite in a eutectic reaction, where the local composition, cooling- and inoculation conditions determine the morphology of the graphite as well as the size of the eutectic cells [2, 3]. These features have been studied and correlated to both mechanical and physical material properties in several works. The elastic and plastic behaviour is influenced by graphite
morphology [4], but also the metal matrix where a smaller eutectic cell size [5] and a denser primary dendritic network [6] has been associated with increasing ultimate tensile strength (UTS). In addition, a higher cooling rate in the subsequent solid-state transformation of austenite to pearlite refines the lamellar spacing of the pearlite, which also contributes to increased material strength with respect to plastic deformation [7]. In addition to microstructure-based variations in mechanical properties, the temperature dependency of both elastic and plastic tensile and compressive properties has been investigated and shown to vary significantly e.g. by Maraveas et al. [8]. Holmgren, Dioszegi and Svensson investigated the connection between thermal conductivity, carbon content and solidification conditions, and found that there exist linear relationships between thermal conductivity and the carbon content, carbon equivalent as well as the fraction of former primary austenite which transforms into pearlite [9]. More specifically, a slower cooling rate leads to a higher tendency for straight, long graphite flakes and a high thermal conductivity, while a faster cooling rate leads to an increased fraction of primary austenite and a decreased thermal conductivity [10]. The difference in thermal conductivity has also been found to be higher at room temperature and decreasing with increasing temperature [9].

A simulation strategy has previously been presented [11] which aims to predict and consider local variations of elasto-plastic material behaviour in FEA, based on microstructural features predicted by casting process simulations. The strategy, denoted the closed chain of simulations for cast components has been evaluated for both ductile iron and cast aluminium components, revealing that the local variations may significantly affect the distribution of stresses and strains when the casting is subjected to load [12]. The approach has been limited to temperature independent mechanical properties, which has prevented it from predicting the performance of components such as engine blocks and cylinder heads, where temperature dependence and physical properties are important aspects to consider. Furthermore, cast irons exhibit a strength-differential effect, i.e. the plastic material behaviour differs significantly between tensile and compressive loading [13], which has not been considered previously. The current work aims to extend and improve the simulation strategy by enabling consideration of temperature dependent mechanical and physical properties and the strength-differential effect of the material. The methodology is demonstrated on a cast iron cylinder head, which has been investigated experimentally for mechanical and physical property variations. In the current work, local material properties are directly linked to the solidification time of the cast material, an approach which has previously been successfully applied for mechanical properties by Ferro et al. [14]. The integrated simulation methodology presented in this work is relevant to design engineers, production engineers as well as material scientists, in order to study and better understand the influence local microstructural variations has on the performance and behaviour of cast components under in-use conditions.

2. Methods

2.1. Experimental procedure
Physical and mechanical testing was performed in order to evaluate the temperature dependent material properties at various locations throughout the studied component. Tensile and compression testing was performed, as well as Differential Scanning Calorimetry (DSC), Laser Flash Analysis (LFA), thermal expansion using a dilatometer and density using Archimedes principle. The sample extraction points are illustrated in Figure 1 and were selected based on solidification time as predicted by a casting process simulation, with the aim of finding regions with different microstructural characteristics. Two characteristic solidification times were selected which will be referred to as "fast" and "slow" solidification in the following analysis and correspond to thinner and thicker sections of the casting. Further details regarding the experimental investigation will be presented in an accompanying work.
2.2. Material data modelling
The non-linear mechanical material behaviour was modelled using Hollomon's equation, \( \sigma = K \varepsilon_{pl}^n \), where the flow stress \( \sigma \) (MPa) is given in terms of plastic strain \( \varepsilon_{pl} \), and the strain hardening parameters \( n \) (-) and \( K \) (MPa). Curve-fitting was performed using a Hooke and Jeeves search pattern-based optimization algorithm, where the difference between experimental stress-strain curves and Hollomon's equation is minimized until \( n \), \( K \) and Young's modulus are found [15]. This methodology allows the modelling and expression of the elasto-plastic material behaviour in terms of microstructure or solidification time. Linear material data models on the form \( f(t) = A(Bt + C) \) were created based on the optimization results, where \( t \) (s) is the solidification time from casting process simulations, \( A \) is a simple temperature scaling factor based on the data presented by Maraveas et al. [8], \( B \) is the change in property per second of solidification time and \( C \) is the base property value at 200 seconds solidification time. Models for temperature dependent thermal expansion, density and specific heat were extracted from the experimental data in the same way.

2.3. Simulations
The MAGMAiron™ module of MAGMASOFT™ version 5.3.1 was used in order to study the heat extraction and microstructure evolution of the cylinder head during the casting process. Only solidification was simulated. The chemical composition of the cast alloy and the sand mould was provided by the cylinder head manufacturer. A temperature dependent Heat Transfer Coefficient was used between sand mould, cooling plates and the cast component. The MAGMAlink™ module of MAGMASOFT™ was then used in order to map the solidification time to each element of a structural mesh consisting of approximately 300 000 first order tetrahedral elements. The overall methodology is illustrated principally in Figure 3.

The static thermomechanical and transient thermophysical behaviour of the cylinder head was studied using Abaqus™ 6.14.3. An in-house Python code was applied in order to generate element
specific material properties, based on the results of the casting process simulation. The code is an extension of what has previously been presented by Olofsson and Svensson in [11]. The main difference is that we now also consider local variations and temperature dependency in density, elasticity, plasticity and thermal conductivity, as well as the strength-differential effect, i.e. that both elastic and plastic material behaviour differs depending on if the local stress state is tensile or compressive. In order to reduce the complexity of the simulation model, a reduction of the number of material definitions was performed. This reduction is based on a small tolerance, where elements with similar material properties are grouped together using the same material definition. By letting the Young's modulus, Hollomon parameters and thermal conductivity vary using 100 discrete values each, the initial element specific material definitions were reduced down to a total of 1750. The influence of this simplification has previously been investigated and demonstrated to be low [12].

A transient thermal analysis was performed using a temperature load of 400°C applied to all cylinder surfaces during 5000 seconds in order to reach thermal equilibrium. The temperature field of the complete geometry was compared to an identical model using only one homogeneous material definition. This homogeneous material definition was taken as the average of the initial 300 000 element-specific properties, i.e. based on the variation established experimentally, and therefore a very good approximation. The same comparison was made with and without material property temperature dependency. A series of static analyses were performed using the same methodology, where a pressure linearly increasing from 0 to 150 MPa was applied to all cylinder surfaces. In these models, the variables are material homogeneity, temperature dependency of material properties and inclusion of compressive material data, which resulted in $2^3$ combinations and models. The stress-field difference was then analysed by successively subtracting simulation results from the each other.

3. Results and Discussion

3.1. Material properties

The results from the physical property testing are presented in Table 1. Figure 4a shows the compressive strength of the material as measured from one sample, suggesting that the ultimate compressive stress (UCS) increases with the refinement of microstructural features caused by a lower solidification time, in agreement with Sjögren [4]. The apparent UCS of 700 - 950 MPa and maximum compressive strain of approximately 10% may be compared to the Ultimate Tensile Strength (UTS) of 180 - 220 MPa and 0.7% tensile failure strain from the same alloy and component. These values are also in agreement with findings from Maraveas et al. [8]. The Coefficient of Thermal Expansion (CTE), the density $\rho$ and the specific heat $C_p$ were not found to be significantly influenced by solidification time and are therefore presented as one value per temperature. Thermal conductivity however was found to increase with
increasing solidification time at all measured temperatures, which is illustrated in Figure 4b. The difference is in agreement with previous findings such as Holmgren [10]. Previous studies [9] have however found the difference in thermal conductivity between solidification conditions to be larger at room temperature than at elevated temperatures, which was not seen in the current study. The coefficient of thermal expansion and specific heat were found to increase with temperature, while density decreased.

Table 1. Temperature dependency of the coefficient of thermal expansion CTE, density ρ, specific heat $C_p$, thermal conductivity $\lambda$ for slow (1800 s) and fast (200 s) solidification. Values are given with an error of one standard deviation.

| Temperature (°C) | CTE (µm/(m°K)) | ρ (kg/m$^3$) | $C_p$ (J/(kg*K)) | $\lambda_{slow}$ (W/(m*K)) | $\lambda_{fast}$ (W/(m*K)) |
|------------------|-----------------|--------------|------------------|--------------------------|--------------------------|
| 25               | 10±0.79         | 7300±19      | 470±3.1          | 49±0.23                  | 48±0.20                  |
| 100              | 12±0.29         | 7200±19      | 510±4.0          | 47±0.35                  | 46±0.14                  |
| 300              | 15±0.14         | 7200±19      | 600±1.1          | 43±0.49                  | 42±0.19                  |
| 400              | 15±0.57         | 7100±19      | 640±3.2          | 41±0.56                  | 40±0.08                  |
| 500              | 16±0.72         | 7100±19      | 700±6.7          | 40±0.46                  | 38±0.17                  |

3.2. Simulation results
The process simulation predicts solidification times between 200 and 1800 s for different regions of the cylinder head. A cross-sectional view of the component is given in Figure 2. It is noted that most of the volume, which is under both thermal and mechanical load, solidifies slowly, i.e. a solidification time above 1000 s. It should also be pointed out that the geometry presented in this work is a simplification of the actual component due to confidentiality.

To evaluate the influence of the different types of material data on the FEA simulation results, the model containing all the available data was set as the reference. Comparisons were then made where the results of the other models with reduced material data are subtracted from the reference model. The error in von Mises stress, taken as the difference between the reference and the reduced model is summarized in Table 2. Also, the difference in the predicted temperature field was evaluated in the same way. The comparison between models containing homogeneous (one material definition) and heterogeneous microstructure-based material properties shows only a small difference in stress of about 5 MPa. This is explained by the very small difference in microstructure in the volume under stress. The second comparison was made between models using temperature dependent data versus room temperature data using an elevated ambient temperature of 500°C. By neglecting temperature-dependency, one under-estimates the local stress by 23 MPa (30%), and over-estimates it by 27 MPa (42%) in other regions. If the strength-differential effect is not considered, the stress is under-estimated by 82 MPa (69%) in some
regions, while it is over-estimated in other regions by 30 MPa (50%). For all of these comparisons, the error distribution was found to be non-intuitive, i.e. it is not distributed with any intuitive pattern with respect to the load-case.

Table 2. Comparison of the difference in von Mises stress and temperature obtained in the FEA simulations when different types of material data is removed.

| Removed data                  | $\Delta \sigma_{vM,\text{under}}$ (MPa) | $\Delta \sigma_{vM,\text{over}}$ (MPa) | $\Delta T_{\text{under}}$ (°C) | $\Delta T_{\text{over}}$ (°C) |
|-------------------------------|----------------------------------------|---------------------------------------|-------------------------------|------------------------------|
| Heterogeneous distribution    | 4.7                                    | 3.6                                   | 0.29                          | 0.04                         |
| Temperature dependency        | 23                                     | 27                                    | 51                            | 17                           |
| Strength-differential effect  | 82                                     | 69                                    | 30                            | 50                           |

Regarding temperature distribution, the difference between homogeneous and heterogeneous simulation models was found to be very small, 0.3°C (0.08%). Again, this is explained by the high level of microstructural homogeneity in the evaluated part of the current casting. If the temperature dependency of the material data is ignored, an overestimation in temperature of 51°C (17%) at the outermost surface from the applied temperature load was seen. In this case the error in temperature distribution is much more intuitive, increasing with distance from the applied load.

4. Conclusions
By evaluating and comparing simulation models with varying degrees of material heterogeneity, it was shown that small errors are introduced by neglecting the microstructural differences due to the casting process in the studied component. Much larger errors are introduced by neglecting the strength-differential effect or the temperature-dependency of the material properties. The error distribution is also non-intuitive in most cases, highlighting the relevancy of the method. While these conclusions are specific to the studied component, load-cases and casting conditions, it should be noted that the methodology been is general to any load-case, geometry or even manufacturing process which induces variations in material behaviour, i.e. not necessarily limited only to cast components.

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