Simulation of Microstructure-based Mechanical Behaviour of Cast Components

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ABSTRACT

In the process of developing cast iron and cast aluminium components, a high level of co-operation between product development and production is of great importance. From an engineering standpoint, this co-operation is limited early in the product development phase by e.g. a lack of established methods for the consideration of local variations in the mechanical behaviour of a finished component.

This thesis aims to increase the possibilities for co-operation between product development and production during the product realisation process by introducing and studying the use of predicted local mechanical behaviour in structural analyses of cast components. A literature review of existing simulation methods and a work on characterisation of mechanical behaviour from microstructural features have been performed to identify important knowledge gaps. A simulation strategy has been formulated which is able to predict local mechanical behaviour throughout the entire component, and to incorporate this into a Finite Element Method (FEM) simulation of the structural behaviour of the component. In the simulation strategy, component-specific microstructure-based mechanical behaviour is predicted using a casting process simulation. A computer program was developed to create FEM material definitions which capture the local variations in mechanical behaviour throughout the component. Using a material reduction technique, the local mechanical behaviour can be incorporated without increasing the FEM simulation time.

The relevance of the simulation strategy was experimentally verified on cast aluminium samples, where the strain field was observed using Digital Image Correlation (DIC). It was found that the local variations in mechanical behaviour cause a stress-strain distribution that deviates from that predicted by a homogeneous material description, indicating the importance of calculating with and including such variations in material behaviour in FEM simulations. Numerical investigations demonstrate the strategy’s relevance for predicting the behaviour of cast aluminium and ductile iron components.

Keywords: Component behaviour, structural analysis, mechanical behaviour, casting process simulation, Finite Element Method (FEM) simulation.
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SUPPLEMENTS

The following supplements constitute the basis of this thesis.


Olofsson was the main author. Larsson performed the experimental work. Svensson contributed with advice regarding the work.


Olofsson was the main author. Svensson contributed with advice regarding the work.


Olofsson was the main author and presented the work at Modelling of Casting, Welding and Advanced Solidification Processes XIII (MCWASP XIII) in Schladming, Austria, 17-22 June 2012. Svensson contributed with advice regarding the work.


Olofsson was the main author. Svensson contributed with advice regarding the work.
Supplement VI  

Olofsson was the main author and presented the work at The 3rd International Symposium on Cutting Edge of Computer Simulation of Solidification, Casting and Refining (CSSCR 2013) in Helsinki, Finland, 20-23 May 2013. Svensson contributed with advice regarding the work. Sample preparation, optical microscopy and tensile testing was performed by a M.Sc. student.

Supplement VII  

Olofsson was the main author and performed the experiments. Svensson contributed with advice regarding the work. Lava and Debruyne contributed with DIC software, experimental setup guidance and reviewing of the manuscript.

Supplement VIII  

Jarfors was the main author and presented the work on Processing and Fabrication of Advanced Materials XXII (PFAM XXII) in Singapore, 18-20 December, 2013. Seifeddine contributed with sections on microstructure and the consequences of defects. Olofsson contributed with a section on modelling and simulation of mechanical behaviour of components and performed simulations and evaluations. Svensson contributed with advice regarding the work and reviewing of the manuscript.
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CHAPTER I

INTRODUCTION

CHAPTER INTRODUCTION

The background for the current work is described, followed by an outline of the theory behind the mechanical behaviour of cast aluminium and cast iron components.

1.1 BACKGROUND

As the demand increases for development processes facilitating the development of cast components with e.g. high strength, low weight, and high reliability, in a short time and at a low cost, as in e.g. the automotive and transportation industries, the effectiveness of the product realisation process becomes increasingly important. The significance of co-operation between product development and production on the industrial organisational level has been emphasised by several researchers [1-4]. Product designers need to take production aspects into consideration already during the design phase of the product realisation process, and production should be considered as an integrated part of this process rather than simply producing whatever is 'thrown over the wall' [1, 2]. The suitability of the product development/production interface is important, and upstream sharing of information between departments has been identified as a critical factor for the success and effectiveness of product realisation projects [3, 4].

Figure 1: Upstream sharing of information in a stage of the product realisation process for a cast component.
On the engineering level, integration between product development and production may be limited by e.g. the mutual dependency between design and manufacturing aspects. In the early design phase of a cast component, the design department uses e.g. virtual computer aided design (CAD) models and computer aided engineering (CAE) tools as finite element method (FEM) simulations in order to predict the behaviour and performance of the component. The inputting of the correct data regarding material behaviour in the virtual component is crucial to the accuracy of these predictions. The actual material behaviour in the real cast component, however, is determined by local casting process conditions, which in turn depend upon both component design and casting process parameters. Material behaviour will thus be component- and design-specific, with local variations to be found throughout the final piece, and there is a mutual dependency between design and production aspects in the behaviour of the component. This mutual dependency should be taken into consideration in the design phase, but is typically avoided by assuming homogeneous material behaviour from standard or tabulated data in the FEM simulation. This assumption, however, is an over-simplification which introduces an unknown quantity of error into the FEM simulation, and limits the transfer of information between production and product development during the product realisation process.

Casting process simulation software has become an established tool for performing virtual casting of components in order to e.g. verify castability and quality at a late stage of the product realisation process, commonly either at the production department or at the foundry. However, the recent development of casting process modelling tools has enlarged the functionality of the software so as to allow it to accurately predict local microstructure formation and variations in material behaviour throughout the cast component [5, 6]. If this information regarding local material behaviour could be transferred upstream in the product realisation process to the FEM simulations in the design phase, as illustrated in Figure 1, the work of design engineers, CAE engineers, and material or foundry engineers could be integrated earlier during the product development process. This would be beneficial to the fit of the product development/production interface, and it is also expected to increase both the ability of FEM simulations to accurately predict the true behaviour of cast components and the effectiveness of the product realisation process.

1.2 MECHANICAL BEHAVIOUR OF CAST COMPONENTS

1.2.1 Theoretical background

The mechanical behaviour of a material subjected to a load is commonly characterised using a stress-strain curve, which is achieved by performing a uniaxial tensile test. The stress-strain curve shows the engineering stress, $s$, versus engineering strain, $e$. For many materials used in engineering contexts, a fairly linear elastic behaviour can be identified at stress levels below the yield stress, followed by a non-linear plastic behaviour at stress levels above the yield stress (see Figure 2a). It is often difficult to identify the yield stress that corresponds to zero plastic strain, meaning that an offset yield stress corresponding to a certain amount of plastic strain, typically 0.2%, is used. In this thesis, the term yield strength (YS) refers to the 0.2% offset engineering yield stress, $s_{0.2}$, while ultimate tensile strength (UTS), $s_u$, is
the largest engineering stress the material can withstand, and fracture strain, $e_f$, is the total engineering strain at fracture, commonly referred to as the ductility of the material.

In order to take into consideration the change in cross-sectional area during deformation, the measures of true stress and true strain are introduced. True stress, $\sigma$, is related to engineering stress and engineering strain through the relationship $\sigma = s(e+1)$; true strain, $\varepsilon$, is related to engineering strain through $\varepsilon = \ln(e+1)$ [7]. The true total strain is the sum of the contributions of true elastic strain, $\varepsilon_{el}$, and plastic strain, $\varepsilon_{pl}$, i.e.

$$\varepsilon = \varepsilon_{el} + \varepsilon_{pl}$$  \hspace{1cm} (1)

The derivative of the true stress-true strain curve is known as the strain hardening rate, $\theta$. The elastic strain is commonly related to stress through Hooke's law, which characterises the linear elastic region using Young's modulus, $E$, as

$$\sigma = E \cdot \varepsilon_{el}$$  \hspace{1cm} (2)

Several different models have been proposed to characterise the plastic behaviour [8]. In this thesis, the Hollomon and Ludwignon equations are used. The Hollomon equation [9] relates true stress and true plastic strain, $\varepsilon_{pl}$, as

$$\sigma = K_H \cdot \varepsilon_{pl}^{n_H}$$  \hspace{1cm} (3)

where the material constants $n_H$ and $K_H$ are introduced. The strain hardening exponent, $n_H$, defines the work hardening capacity of the material, and ranges from zero to one, where $n_H = 0$ corresponds to a perfectly plastic material, in which $\sigma = K_H$ and $n_H = 1$ corresponds to a linear deformation hardening material where $\sigma = K_H \cdot \varepsilon_{pl}$. Metallic materials commonly fall within the range of $n_H = 0.1$-0.5, values which correspond to different shapes of the plastic curve as shown in Figure 2b.

![Figure 2](image-url)

(a) Basic definitions of tensile properties. (b) Effect of different values of the strain hardening exponent, $n_H$, on the shape of the plastic stress-strain curve predicted by the Hollomon equation (Eq. 3).
For ductile materials, the strain hardening exponent also measures the maximum uniform strain, and numerically corresponds to the true plastic strain at necking [7, 10]. The constant commonly referred to as the strength coefficient, \( K_H \), can be expressed as a function of yield stress and the strain hardening exponent [7]. To determine the constants \( n_H \) and \( K_H \) from a tensile curve, a double logarithmic plot of true stress and true plastic strain is used. If the plastic behaviour of the material follows the Hollomon equation, such a plot yields a straight line where \( n_H \) is the slope of the line and \( K_H \) is the stress level when the true plastic strain equals unity.

For some materials, a double logarithmic plot shows a two-slope behaviour, with one slope for small plastic strains and one for larger strains [11, 12]. The Ludwigson equation [11] (Eq. 4), extends the Hollomon equation to correct for this behaviour by introducing an exponential correction term which gives a correctional contribution for small plastic strains which diminish at higher levels of strain.

\[
\sigma = K_H \cdot \varepsilon_p^{n_H} + \exp\left(k_L + n_L \cdot \varepsilon_p\right) \quad (4)
\]

The correction term may be positive or negative, depending on material behaviour, and introduces two additional material constants, \( k_L \) and \( n_L \), determined by plotting the natural logarithm of the error between the measured true plastic strain and the true plastic strain as predicted by the Hollomon equation. For small plastic strains, a linear region can be identified where \( n_L \) is the slope of the line and \( k_L \) is the interception point when the plastic strain equals zero.

In multi-axial stress conditions, the stress state is described by the stress tensor \( \sigma_{ij} \) from which three principal stresses, \( \sigma_1-3 \), can be determined. Respectively, the hydrostatic stress, \( \sigma_h \) (Eq. 5), and the von Mises equivalent stress, \( \sigma_{VM} \) (Eq. 6), are defined as [13, 14]

\[
\sigma_h = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3) \quad (5)
\]

\[
\sigma_{VM} = \frac{1}{\sqrt{2}}\left\{ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right\} \quad (6)
\]

In the von Mises yield criterion, yielding is assumed to occur at the point when the von Mises stress exceeds the yield stress of the material, derived in uniaxial tension [13]. The stress tensor can be expressed as the sum of the hydrostatic stress tensor, which tends to change the volume of the body, and a stress deviator tensor, \( S_{ij} \) (Eq. 7), which tends to distort it. In tensor notation form, the stress deviator tensor can be expressed as [14]

\[
S_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \quad (7)
\]

where \( \delta_{ij} \) is the Kronecker delta, i.e.

\[
\delta_{ij} = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j 
\end{cases}
\]

The second invariant of the stress deviator tensor, \( J_2 \), is given as [14]

\[
J_2 = \frac{1}{2} S_{ij} S_{ij} \quad (8)
\]
1.2.2 Mechanical behaviour of cast aluminium alloys

The mechanical behaviour of cast aluminium alloys is determined by both the microstructure and the defects obtained during the casting process. These alloys typically contain several alloying elements in addition to aluminium. The main alloying element is silicon (Si), which comprises 5-15% and improves strength and castability. Lesser amounts of e.g. copper (Cu), iron (Fe) and magnesium (Mg) may also be added to alter the characteristics of the material. During the solidification of a hypoeutectic alloy (containing less than 12% Si), pure aluminium (Al) in a dendritic shape is the first phase to solidify, assuming a low content of other alloying elements. The distance between the dendrite arms is known as the Secondary Dendrite Arm Spacing (SDAS); see illustration in Figure 3a. During the subsequent eutectic solidification, both Si particles and dendritic Al precipitate. In hypereutectic alloys (>12% Si), Si particles precipitate before the eutectic solidification begins. In the following, a few of the features which affect the mechanical behaviour of cast aluminium alloys will be introduced briefly.

1.2.2.1 Cooling rate

The local cooling rate during solidification is determined by the design of the component, and by the process conditions. In general, a thick section gives a lower cooling rate than a thin one. Higher cooling rates refine the microstructure through e.g. a smaller SDAS [15, 16], and refine the eutectic Si-particles [17]. This is seen in Figure 3, where the microstructure of a cast aluminium alloy is shown, first with a high cooling rate in Figure 3a-b, and then with a low cooling rate, Figure 3c. In Figure 3a-b, there are white dendrites with an SDAS of approximately 8 μm, and the Si particles are merely seen as grey dots in the eutectic regions between the dendrites. In Figure 3c, the dendrites are significantly larger, with an SDAS of approx. 50 μm, and the Si particles may be clearly seen as large, dark grey particles. Higher cooling rates also strengthen the dendrites due to Si-enrichment [18]. YS generally increases with higher cooling rates for as-cast materials [18-20], but the effect is reduced or non-existent for heat treated alloys [17, 21, 22], since the strengthening effect of the Si-enrichment of the dendrites is removed by homogenisation of the alloying elements during heat treatment [18]. UTS and ductility is highly related to the coarseness of the microstructure, and generally increases with higher cooling rates [15-19, 21-23]. However, these trends may have variations due to concurrent changes in the size and shape of the eutectic Si particles [22, 24].

1.2.2.1 Structural integrity

The mechanical performance of cast aluminium alloys is highly related to structural integrity, including defects such as e.g. porosity and oxide films. Porosity, exemplified in Figure 3b, may be caused by e.g. entrapped gas or solidification shrinkage [25]. Oxide films, which form on the surface of the liquid, melt and become entrained in the liquid during the casting process, forming a non-load bearing area within the solid metal [25]. Structural integrity particularly affects UTS and ductility, both of which decrease with increased levels of porosity [25, 26]. YS, however, remains relatively unaffected, because small reductions in the load bearing area are counteracted by local yielding and strain hardening [25-27].
1.2.2.2 Si content and Si particle morphology

Increasing the Si content in the hypoeutectic region increases the volume fraction of the eutectic phase, which is hard and strong. This leads to increased UTS but decreased ductility. In hypereutectic alloys, UTS continues to improve with increasing Si content up to 16%, but decreases as the Si content is increased further after this point [28]. The morphology, distribution, and damage to the Si particles [29-33] dominate the strain hardening behaviour of the alloy [34]. Damage to the Si particles is caused by incompatibility stresses between particle and matrix, where the local maximum principal stress causes the fracture of Si particles, while tensile hydrostatic stress (c.f. Eq. 5) drives debonding [35]. Changing the morphology of the Si particles from acicular to fibrous, through chemical or thermal treatment, increases the strength between matrix and particles, which in turn increases ductility and strain hardening rate [33, 36-38].

1.2.2.3 Fe-rich phases

Fe-rich phases, most importantly α-, β- and π-Fe phases, are common in cast aluminium alloys containing iron (Fe). In Figure 3c, Fe-rich phases are seen as light grey lines of varying length and thickness. These phases are detrimental to the mechanical properties, especially the β-Fe plates, which induce stress concentrations and decrease ductility [39]. Simultaneous alloying with a sufficient quantity of manganese is recommended in order to suppress the formation of β-Fe plates in favour of the less harmful α-Fe phase. However, the actual size and area fraction of β-Fe phases are also affected by the local cooling rate [18].

![Figure 3: Microstructure of a cast aluminium alloy using (a-b) high cooling rate (SDAS ~8 μm) and (c) low cooling rate (SDAS ~50 μm). Illustration of SDAS (1), porosity (2), Si-particles (3) and Fe-rich phases (4).](image)

1.2.3 Mechanical behaviour of cast irons

The term 'cast iron' is used to identify a large family of ferrous alloys with a carbon content which, in the binary case, is higher than 2%. The traditional classification of cast irons splits samples into two groups, based on the colour of the fracture surface of the material (grey iron and white iron) [40]. Today, however, cast irons are instead distinguished according to their graphite morphology and metal matrix structure. In a similar manner to cast aluminium alloys, several microstructural features affect the
mechanical behaviour of the material. In the following, the influence of different graphite morphologies and metal matrices will be briefly introduced.

1.2.3.1 Graphite morphology

The following graphite morphologies, shown in Figure 4, are discussed in the current work:

- **Flake graphite iron (FGI)**, also called grey iron or lamellar graphite iron.
- **Compacted graphite iron (CGI)**, also known as vermicular graphite iron.
- **Spheroidal graphite iron (SGI)**, commonly referred to as ductile iron (DI), or nodular cast iron.

![Graphite morphology](image)

**Figure 4: Graphite morphology of (a) FGI (b) CGI and (c) SGI [40].**

Graphite morphology significantly affects the mechanical behaviour of cast irons with similar matrix compositions. FGI exhibits no linear elastic region, as well as a low Young’s modulus and reduced strength. In CGI, a seemingly linear elastic region with a higher Young’s modulus and increased strength is obtained. SGI exhibits an essentially linear elastic region, with a higher Young’s modulus and even higher strength. The Young’s modulus can be described as a function of the nodularity and aspect ratio of the graphite particles [41], although no cast iron grade exhibits perfectly linear elastic behaviour, and plastic deformation occurs already in the seemingly linear elastic region [42]. The effect of graphite morphology is commonly attributed to the shape of the graphite particles, where the sharp edges of the graphite lamella in FGI cause large local stress concentrations and immediate plastic deformation during tensile loading [42]. It has been pointed out, however, that this reduction in strength is caused primarily by the interconnection between the graphite particles which, due to their being closely packed within the matrix of FGI, decrease the length of the crack propagation path through the matrix, thus causing rapid crack propagation [43]. In CGI, the graphite lamella has a blunter shape, causing fewer local stress concentrations, and the lesser graphite continuity gives a more lengthy crack propagation path within the matrix. Thus, the yielding properties are to a larger extent governed by the metal matrix in CGI than in FGI. The graphite nodules with a rounded shape which are found in SGI cause the least local stress concentrations and graphite continuity in the matrix, thus resulting in the highest strength [42-44]. Graphite morphology is controlled by alloying, but is also affected
by the local cooling rate. Component geometry thus affects the behaviour of the material throughout a cast iron component [40].

1.2.3.2 Metal matrix

The metal matrix commonly consists of ferrite, pearlite, or a combination of both. The ferrite structure has low strength and high ductility [45], and increasing the size of the ferrite grains causes a small decrease in tensile strength, of the strength coefficient, and of the strain hardening exponent [46]. Pearlite is a lamellar structure of ferrite and cementite which is hard and brittle, and the strength of a pearlitic matrix is reported to be dependent on alloying, strengthening from interlamellar spacing, and pearlite colony size [40]. The interlamellar spacing is determined largely by the local cooling rate, where a high cooling rate gives a smaller interlamellar distance [40, 45]. Both the strength coefficient and the strain hardening exponent increase with decreasing interlamellar spacing [46]. The cooling rate also affects the amount of ferrite and pearlite in the matrix [40], and thus matrix strength is dependent on the local geometry throughout the component.

Similar to cast aluminium alloys, cast irons may also be heat treated. In this thesis, the austempering heat treatment process will be discussed. This consists of two steps; austenitising and austempering. In the former, the material is heated to the austenitising temperature and held there until the matrix is fully austenitised. Following this, the material is quenched to the austempering temperature, which is maintained until the austenitic matrix is transformed into a matrix called ausferrite, consisting of acicular ferrite and austenite [47]. The austempering heat treatment is most commonly applied to ductile iron, SGI, and the resulting material is denoted austempered ductile iron (ADI). Increases in various material properties, such as strength, wear resistance, toughness, or fatigue strength, can be achieved by correctly selecting the parameters of the heat treatment, e.g. austempering temperature and duration [48, 49]. This makes ADI a very attractive material that, in certain applications, may replace steel, e.g. components for earth-moving equipment [49].

1.2.4 Predicting the mechanical behaviour of cast components

As previously described, the microstructure formation within a cast aluminium or cast iron component is affected by complex interactions between component design, chemical composition, casting process parameters, and, where applicable, post-solidification treatment. These factors do not affect all parts of a component to the same extent during the casting process, which causes local variations in microstructure and, due to the fact that the microstructure determines mechanical behaviour, the cast component itself will display local variations in mechanical behaviour. Thus, a cast component exhibits a heterogeneous, as opposed to homogeneous, material behaviour. To be able to predict the behaviour locally throughout a cast component, numerical modelling of the formation of the microstructure within the component during the casting process is essential.

The modelling of microstructure formation during solidification can be performed on different scales, e.g. macroscopic (i.e. the level of the entire process), microscopic (basic microscopic mechanisms such as nucleation and growth of phases), mesoscopic (grains), or combinations of the above, such as micro-macroscopic or
multi-scale models [50]. The modelling approaches are either deterministic or stochastic in nature, although coupled deterministic-stochastic approaches have been presented [51]. Computer-based approaches for the modelling of the solidification of cast irons originate in the work of Oldfield in 1966 [52], and have since been much developed through the work of e.g. Fredriksson and Svensson [53] and Su et al. [54] in 1985. As computer technology has evolved, models have been further extended, and numerical techniques for modelling microstructure formation throughout both cast iron and cast aluminium components have been developed [55, 56]. These models have commonly been combined with casting process simulation software in order to predict microstructure evolution throughout an entire component. In casting process simulation software, chemical composition and casting process parameters are defined, and the entire casting process itself can be simulated, from mould filling to solidification, solid-state transformations, and possible heat treatment. The software is also able to predict residual stresses, i.e. those that form within a component as a result of the contraction of the casting as it cools to room temperature, and that remain within the component after the casting process [25].

Using material characterisation models, the predicted microstructure can be applied to predict the mechanical behaviour of the material throughout the component. For an as-cast aluminium alloy, Seifeddine et al. [57] used the local value of SDAS predicted by a casting process simulation to predict the local variations in YS, UTS, and ductility of a cylinder head component, all of which transpired to be in good agreement with experimental data. The parameters of the Hollomon equation (Eq. 3) i.e. the strain hardening exponent, \( n_H \), and the strength coefficient, \( K_H \), were found to be highly related to the local Fe content and the value of SDAS. Relationships for the parameters have been derived (Eqs. 9-10) as; [58]

\[
\begin{align*}
    n_H &= (a_1 \cdot \text{Fe} + a_2) \cdot \ln(\text{SDAS}) + (a_3 \cdot \text{Fe} + a_4) \\
    K_H &= (b_1 \cdot \text{Fe} + b_2) \cdot \ln(\text{SDAS}) + (b_3 \cdot \text{Fe} + b_4)
\end{align*}
\]

where \( a_{1-4} \) and \( b_{1-4} \) are the respective constants derived from tensile testing. Similar models are also being developed for heat-treated aluminium alloys [59].

For cast irons, models for predicting the Young’s modulus based on graphite morphology have been derived and applied to simulations of a CGI engine block [41, 60]. The influence of microstructural properties on plastic behaviour has been investigated [5, 12, 46, 61, 62] and, for FGI and CGI, the Hollomon equation (Eq. 3) was found to accurately predict the plastic behaviour, while the Ludwigon equation (Eq. 4) was found to yield more accurate results for SGI [12]. Relationships for the parameters have been derived (Eqs. 11-14) which take into account the local pearlite and graphite content; [12]

\[
\begin{align*}
    n_H &= c_1 \cdot (\text{PEARLITE\%}) + c_2 \\
    K_H &= d_1 \cdot (\text{PEARLITE\%}) + d_2 \\
    n_L &= \exp(e_1 \cdot (\text{ROUNDNESS}) + e_2) \\
    k_L &= f_1 \cdot (\text{NODULARITY}) + f_2
\end{align*}
\]
where \( c_{1-2}, d_{1-2}, e_{1-2} \) and \( f_{1-2} \) are constants derived from tensile testing.

The relationships expressed in Eqs. 9-14 have been implemented into a development version of a commercial casting process simulation software in order to enable the prediction of parameter values for the Hollomon or Ludwigson equations throughout a cast component. These predictions are based on the predicted local microstructure and are referred to as \textit{microstructure-based mechanical behaviour} in this thesis.
CHAPTER 2

RESEARCH APPROACH

CHAPTER INTRODUCTION

This chapter describes the research methodology used in this thesis. The purpose and aim of the thesis are described first, followed by a description of the research design. The materials and the practical and numerical experimental procedures are then introduced.

2.1 PURPOSE AND AIM

The primary purpose of this work is to increase the usability of casting process simulations and material characterisation models in the design process for cast iron and cast aluminium components. For several years, extensive research has been conducted at the department of Materials and Manufacturing – Casting at the School of Engineering, Jönköping University, with the intention of establishing models and simulation tools which predict solidification and microstructural evolution during the casting process, as well as mechanical and physical material behaviour throughout a cast component. These models have been used to extend the functionality of commercially available casting process simulation software by digitally replicating the entire casting process of components and predicting the local mechanical behaviour of a cast component. However, the use of these predictions in structural analyses has been limited, due to the fact that no established method currently exists for utilising the predicted behaviour in FEM simulations.

The aim of this work has been to enable the use of predicted local mechanical material behaviour in FEM simulations of the mechanical behaviour of cast components, and to investigate the effects of local variations in material behaviour on the global behaviour of cast iron and cast aluminium components. This is intended to bring about the use of casting simulations as an integrated part of the simulation-based design process for cast components, thus improving the fit of the product development/production interface, and broadening the possibilities as regards designing cast components with high reliability, performance, and robustness.
2.2 RESEARCH DESIGN

2.2.1 Research perspective

Research can be generally be said to belong to one of two major traditions [63]; the positivist approach or the interpretivist approach. The two approaches are generally associated with different styles of reasoning, namely deductive reasoning and inductive reasoning, respectively. Using deductive reasoning, an argument moves from general principles to particular instances, whereas inductive reasoning begins with particular instances and moves to general statements. The positivist approach is thus associated with deductive reasoning and the testing of hypotheses, while the interpretivist approach is related to inductive reasoning and the generation of working propositions [63].

The traditional positivist research design as stated by Williamson [63] is schematically illustrated in Figure 5. The approach starts with a definition of the topic of interest, followed by the simultaneous creation of a literature review and theoretical framework, as well as a delineation of the research problem and variables. A hypothesis is created and research is performed to collect data, which is analysed and interpreted to see if the hypothesis is supported, leading to a framing of general laws. The positivist approach represents the traditional perspective as regards the natural sciences; it is often related to experimental research designs and quantitative data, and is a fairly linear and fixed framework. The interpretivist approach is comparatively flexible, and tends to be non-linear and iterative, with the researcher able to move between different research activities several times during the process. Qualitative methods of research are typically used, such as case studies and action research [63].

![Schematic illustration of the traditional positivist research design](image)

**Figure 5: Schematic illustration of the traditional positivist research design, as stated by Williamson [63].**

The research approach applied in this thesis is illustrated in Figure 6, and has some similarities to the traditional positivist research design, due to its having an essentially fixed, linear approach. An initial specification of the topic of interest was
defined, a literature review of the research area was performed (Supplement I); this, together with a work on the theory behind the characterisation of the mechanical behaviour of microstructural features (Supplement II), formed the basis for a more detailed definition of the research problem and questions, as well as a definition of the simulation approach. To enable the new simulation strategy, a computer program was then designed and implemented (Supplement III). Three different experimental tracks were followed to analyse, extend, and verify the predicted effects of local mechanical behaviour:

A. Analysis of the simulation strategy for a ductile iron component. Two sets of numerical experiments were performed (Supplements IV-V).

B. Analysis of the simulation strategy for cast aluminium components. Both numerical and physical experiments were performed (Supplements VI & VIII).

C. Extension of material characterisation models for High Pressure Die Cast (HPDC) aluminium, and verification of the predictive power of the simulation strategy using physical observations (Supplement VII).

Figure 6: Schematic illustration of the research approach in the current work.
2.2.2 Experimental design

Experimental research designs can be divided into three broad categories [63]:

- **True experiments**, in which a controlled laboratory setting and the use of a control group (not subject to treatment), an experimental group (subject to treatment), and randomisation, eliminates the potential for disruptive variables.

- **Quasi-experimental designs** use many of the controls in the true experiment, but diverge in that deliberate selections are used, rather than randomisation.

- **Pre-experimental designs** use neither control group, nor control conditions, nor randomisation.

In brief, true experiments make it possible to prove causal relationships, quasi-experimental designs may infer likely causal links but do not prove causality, and, in pre-experimental designs, no meaningful causal links are provided. The use of laboratory settings in a true experiment generally also ensures high internal validity, but the generic applicability of the results to other settings (i.e. the external validity) is low. The internal validity of a quasi-experimental design is much lower than for a true experiment, and, conversely, the external validity is higher [63].

In this thesis, experimental research has been performed due to the fact that causal relationships between quantitative variables were to be established. In the physical experiments performed in Supplement II, two ductile iron alloys were subjected to an ADI heat treatment in a controlled laboratory setting, and an as-cast material that was not subjected to the heat treatment was used as a control group. Precautions were taken to ensure the gathering of accurate measurements, and numerical data evaluation was performed so as to guarantee the reliability of the results. However, as randomisation was not included in the experimental design, it can be considered a quasi-experimental research design, with limited internal validity. Thus, trends can be observed in the data, but these cannot be said to prove causality. On the other hand, external validity for a quasi-experimental research design is generally high, and for each combination of settings, three tests were performed, from which a mean value and standard deviation were determined. The external validity was considered to be sufficient to allow generalisation of the results to the material under investigation, but not enough to create numerical models or generalise the results to all ADI alloys. Similar reasoning can be applied to the experiments in Supplements VI-VII.

The numerical experiments were deterministic in nature. The simulation results are solutions to equations, and are not affected by the order in which the simulations were performed. In addition, repeated simulations which used the same input data lead to identical results, free of statistical variation. Experimental design aspects such as laboratory settings, reliability, randomisation, and statistical probability testing of the results have thus generally not been applicable to the experimental design. In the case of the measurement of simulation times, however, the simulations were repeated to study the obtained variations. Reference simulations which can be regarded as control groups, i.e. not subject to treatment (e.g. material reduction, c.f. Section 3.3.1), have been used. Because of this the experiments can, in a sense, be

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seen as true experiments with high internal validity. General simulation methods have been used, but only one component and one set of casting simulation input parameters have been studied. In Supplements IV-V and VIII, no physical experiments have been performed in order to validate the simulation results against actual components, meaning that external validity is thus limited. In Supplements VI-VII, physical experiments have been performed to validate the numerical results, meaning that the external validity of these experiments is improved.

2.2.3 Literature review

The information gathering process described by Rumsey [64] can be summarised as follows:

- Analysing the question or problem.
- Defining the scope of the research and the information required.
- Identifying sources of information.
- Finding the location of the information.
- Accessing the information.
- Evaluating the information.
- Managing searches and results.
- Updating and monitoring new developments.

This information gathering process includes an online search process, illustrated in Figure 7. The online search process, which is in many ways also applicable to other sources of information, in turn consists of several steps. The first is to plan the search; then, this is performed, and all results of possible relevance to the problem are retrieved and evaluated. If a record is still considered relevant after the evaluation, it is saved and managed. Based on the results of the search, the search plan may need to be modified and some or all of the steps of the search process repeated. If no new relevant records are retrieved, the search process may be considered to be completed [64].

For this thesis, a literature review was performed to obtain secondary data as a foundation for the research work (see Supplement II). An information-gathering process, based on the procedure described above, was used. In the analysis of the problem, the topic of interest was initially broadly defined as 'methods to take the effects of microstructural features of cast irons and cast aluminium alloys into account in structural analyses of components'. Due to the extensive body of information already available on the topic, however, the decision was made to limit the literature review to methods for FEM simulation of mechanical behaviour of cast aluminium components. The scope of the literature review was divided into two parts; the first was concerned with microstructural features which contribute in a significant manner to the mechanical behaviour in cast aluminium alloys, while the second part compares different methods of taking some of these features into
account in FEM-based structural analyses. The information resources used were online databases (primarily ScienceDirect\(^1\), Scopus\(^2\), and SpringerLink\(^3\), but also e.g. journal-specific websites and e-books) and library resources (books and journals). Several iterations of the online search process were developed and used. In addition, citation searching was used, and literature suggestions provided by colleagues were investigated. The relevance of the texts was initially evaluated based on the title and abstract of the records, and the content of those which appeared to be pertinent was then further investigated; records which were felt to still be of relevance after this investigation were then categorised and managed using the EndNote [65] reference management software.

![Figure 7: The online search process according to Rumsey [64].](image)

### 2.2.4 Research questions

Several research questions were raised and addressed at different stages of the research process. The primary questions can be grouped into the following areas, and are addressed to varying degrees in the supplements referenced in brackets.

- **Microstructure and mechanical behaviour (Supplements I, II, VII)**
  - Which microstructural features govern the mechanical behaviour of cast aluminium and cast iron alloys?
  - How may mechanical behaviour be characterised using microstructural features predicted by a casting process simulation?

- **Methodology (Supplements I, III, IV)**
  - What methods exist for taking microstructural features of cast irons and cast aluminium alloys into account in structural analyses of components?
  - How can the predicted local mechanical behaviour be incorporated into FEM simulations?

---

• What is the effect on computational power requirements, i.e. FEM simulation time and data file size? Can the local behaviour be incorporated in such a way that FEM simulation time is not increased?

Effects of local variations in microstructure and material behaviour on component behaviour (Supplements IV-VIII)

• Is the predicted mechanical behaviour of a ductile iron or cast aluminium component affected by the local variations in mechanical behaviour?
  o What is the effect on maximum values of stress and strain?
  o What effect does this have on the distribution of stress and strain throughout the component?
  o Does this effect remain when a consideration of residual stress is added to the simulation?

• Can the effects be confirmed by physical observation?

2.3 MATERIAL AND EXPERIMENTAL PROCEDURES

2.3.1 Materials

2.3.1.1 Ductile Iron

In Supplement II, two ductile irons were investigated. The experimental work was performed by a member of staff at the university. The base materials were cast into ring components with an outer diameter of approximately 0.5 meters, in serial production at two different foundries. The chemical compositions of the as-cast materials are specified in Table 1. The chemical contents were found to be very similar, and no significant difference in the mechanical behaviour of the two alloys was expected.

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mo</th>
<th>Ni</th>
<th>Cu</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADI-1</td>
<td>3.46</td>
<td>2.25</td>
<td>0.37</td>
<td>0.02</td>
<td>0.006</td>
<td>0.04</td>
<td>0.20</td>
<td>0.03</td>
<td>0.78</td>
<td>Bal.</td>
</tr>
<tr>
<td>ADI-2</td>
<td>3.65</td>
<td>2.13</td>
<td>0.34</td>
<td>0.03</td>
<td>0.009</td>
<td>0.04</td>
<td>0.27</td>
<td>0.05</td>
<td>0.82</td>
<td>Bal.</td>
</tr>
</tbody>
</table>

Test specimens were taken from the rings and machined into cylindrical units. These were then subjected to an austempering process, where the austenitising treatment was performed at 900 °C for two hours, and the austempering was performed at four (ADI-1) and five (ADI-2) different temperatures, respectively, and three (ADI-1) and four (ADI-2) different times, respectively; see Table 2.
Table 2: Experimental program for the ADI materials.

<table>
<thead>
<tr>
<th>Austempering temperature</th>
<th>ADI-1</th>
<th>ADI-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>250 °C</td>
<td>1h, 2h, 3h</td>
<td>0.5h, 1h, 2h, 3h</td>
</tr>
<tr>
<td>300 °C</td>
<td>1h, 2h, 3h</td>
<td>0.5h, 1h, 2h, 3h</td>
</tr>
<tr>
<td>325 °C</td>
<td>-</td>
<td>0.5h, 1h, 2h, 3h</td>
</tr>
<tr>
<td>350 °C</td>
<td>1h, 2h, 3h</td>
<td>0.5h, 1h, 2h, 3h</td>
</tr>
<tr>
<td>400 °C</td>
<td>1h, 2h, 3h</td>
<td>0.5h, 1h, 2h, 3h</td>
</tr>
</tbody>
</table>

In Supplements II-V, casting process simulations for a ductile iron component were performed. A ductile iron with the chemical composition found in Table 3 was specified. This composition has previously been used to verify the casting process simulation models [5].

Table 3: Chemical composition in weight per cent (wt. %) specified in the casting process simulations.

<table>
<thead>
<tr>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mo</th>
<th>Ni</th>
<th>Cu</th>
<th>Mg</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.38</td>
<td>3.09</td>
<td>0.34</td>
<td>0.02</td>
<td>0.009</td>
<td>0.04</td>
<td>0.02</td>
<td>0.03</td>
<td>0.29</td>
<td>0.023</td>
<td>Bal.</td>
</tr>
</tbody>
</table>

2.3.1.2 Aluminium

The chemical composition of the aluminium alloy investigated in Supplements VI-VII is detailed in Table 4. The alloy meets the EN AC-46000 standard. In the casting process simulations, 0.6 wt. % Fe was specified due to software limitations.

The base material was sourced from a component taken from serial production at a HPDC foundry. In Supplement VI, component samples for microstructural investigation and tensile evaluation were prepared by a M.Sc. student. In Supplement VII, samples for material characterisation and investigation of local variations in mechanical behaviour were produced by the current author using the gradient solidification technique, in which a furnace is mounted on a motorised lifting device. The layout of the equipment is described in detail elsewhere [66]. The component remainders were initially melted and cast into cylindrical specimens, which were then remelted and solidified in the gradient furnace. Three experimental series with a constant lifting speed of the gradient furnace, generating a SDAS of about 10, 25 and 50 μm, respectively, were produced, here denoted SDAS10, SDAS25 and SDAS50, respectively. One experimental series with accelerating lifting speed was produced, generating a varying SDAS of between 10 and 20 μm over the specimen length. This series is hereafter referred to as the SDASVAR series.

The gradient solidification technique provides controlled and advantageous solidification conditions, and leads to samples of high homogeneity and structural integrity. This makes it possible to study the isolated effect of different solidification microstructures on mechanical behaviour. In a real HPDC process, however, the filling and solidification conditions are more complex, and may lead to e.g. pre-solidified particles, air entrapment, and porosity in the component, all of which affect the mechanical behaviour of the material. The gradient solidification technique is, however, a very useful method for identifying the mechanical potential of the alloy used.
Table 4: Chemical composition in weight per cent (wt. %) of the investigated HPDC aluminium alloy.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Cu</th>
<th>Fe</th>
<th>Mg</th>
<th>Al</th>
<th>Bal.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>9.8</td>
<td>2.7</td>
<td>0.8</td>
<td>0.2</td>
<td>Bal.</td>
<td></td>
</tr>
</tbody>
</table>

2.3.2 Tensile testing

The ADI specimens (Supplement II) were, prior to the heat treatment, machined into cylindrical test bars with a diameter of 7 mm, a gauge length of 50 mm, and a total length of 98 mm. A constant cross-head speed of 0.5 mm/min. was used. For each combination of heat treatment parameters, three tensile bars were tested. Strain was measured using a clip-on extensometer, and the tests were performed by a member of staff at the university.

For the aluminium samples (Supplements VI-VII), flat tensile bars in accordance with standard ASTM: B557M-10 were used, with a specimen thickness of 4 mm, width of 6 mm, and a reduced section length of 32 mm. Tensile tests were performed using a constant cross-head speed of 0.35 mm/min. In Supplement VI, 10 component samples were tested, and the work was performed by a M.Sc. student. For the gradient solidified samples in Supplement VII, six specimens of each series were tested, and the experimental work was performed by the current author. Strain was measured using a laser extensometer, with an initial distance of 26 mm between the measuring points.

All tensile tests were performed at room temperature in a Zwick/Roell Z100 testing machine with 100 kN load capacity.

2.3.3 Digital Image Correlation setup

Digital Image Correlation (DIC) was applied to investigate the strain distribution throughout the gradient solidified aluminium samples in Supplement VII. DIC is an optical non-contact deformation measurement method which enables the measurement of the full displacement and strain fields for a specimen. Typically, a speckle pattern is applied to the specimen under investigation, and during testing the deformation of the speckle pattern is observed by a digital camera. The captured images are then analysed using a DIC algorithm, wherein the full displacement and strain fields are calculated.

In Supplement VII, images were captured by an AVT Stingray F201B 8-bit camera with a Tamron M118FM25 lens (focal length 25 mm). The camera was mounted on the tensile testing device so that one of the flat surfaces was observed, while the laser extensometer irradiated the other. The use of 2D DIC was enabled by the in-plane deformation of the flat specimen and the camera being mounted perpendicular to the specimen. A speckle pattern was applied to the specimens using spray paint, consisting of a matte white bottom layer followed by a second layer of black speckles. Image capturing and correlation was performed using MatchID software [67]. Due to limitations with the experimental equipment, synchronisation with the tensile machine was performed manually. The correlation settings used are shown in Table 5.
Table 5: General parameters used in the DIC correlation

<table>
<thead>
<tr>
<th>Technique used</th>
<th>2D Digital Image Correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Noise</td>
<td>Approximately 1 %</td>
</tr>
<tr>
<td>Subset</td>
<td>15</td>
</tr>
<tr>
<td>Step</td>
<td>5</td>
</tr>
<tr>
<td>Spatial resolution - displacement</td>
<td>15 pixels, about 0.6 mm</td>
</tr>
<tr>
<td>Strain smoothing method</td>
<td>Polynomial - quadratic</td>
</tr>
<tr>
<td>Spatial resolution - strain</td>
<td>71 pixels, about 2.8 mm</td>
</tr>
<tr>
<td>Strain tensor</td>
<td>Logarithmic Euler-Almansi</td>
</tr>
</tbody>
</table>

2.3.4 Simulation procedures

2.3.4.1 Casting process simulation

The component casting processes were simulated using a development version of MAGMASOFT™ [68]. The software uses the Finite Difference Method (FDM), in which the derivatives of the governing partial differential equations are written in terms of finite difference equations [69-71]. In the FDM, the component geometry is traditionally represented by a mesh of rectangular volume elements of regular structure. The use of a structured mesh has the advantages of a low computational cost and a high mesh quality, but the disadvantage of limited representation of irregular geometries. FDM techniques and numerical grid generation approaches, which allow for unstructured meshes, have been developed to overcome this drawback [70-72]. Despite the fact that its limitations make it less suitable for stress analysis simulations [69], FDM is generally considered highly suitable for heat transfer and fluid flow problems in e.g. casting process simulations [70-72].

2.3.4.1 Computer program development

A computer program has been developed which enables the incorporation of predicted material behaviour from the casting process simulation into the stress analysis of the component (see Supplement III). The Python programming language [73] was selected for implementation due to its close integration with ABAQUS™ [74]. The program has been implemented as a plugin for the CAE module of ABAQUS™, and is controlled through a graphical user interface.

2.3.4.2 Component FEM simulation

The stress-strain simulations in this work have been performed using the Finite Element Method (FEM), in which component geometry is represented by a mesh of small finite segments or elements. Different types of elements with various shapes and different characteristics may be used, and the method is able to provide good descriptions of irregular geometries. The size of the elements can be varied in different regions to handle rapidly changing variables, e.g. stress concentrations. FEM is thus suitable for, and well established in, the analysis of solid mechanics [69], but FEM algorithms for the simulation of casting processes are also available [75]. The ABAQUS™ [74] implicit FEM solver has been used. As a result of the fact that the FEM simulation uses a different mesh from that of the casting process simulation, the
results from the latter have been mapped to the FEM mesh using the MAGMALINK™ module of MAGMASOFT™ [68].

The material model used in the current work is an elastic-plastic metal plasticity model, where the linear elastic region is described by Young's modulus and the non-linear plastic behaviour is defined by a piecewise linear curve. The von Mises yield criterion is used, which represents a cylindrical surface in the principal stress space, where only the deviatoric stresses influence the criterion, commonly referred to as $J_2$-plasticity [14] (c.f. Eqs. 7-8). Isotropic hardening is applied, meaning that the yield surface increases uniformly in size as plastic straining occurs [14]. No strain rate or temperature dependency has been included.

2.3.4.1 Tensile test FEM simulation

Tensile test simulations were performed using a three-dimensional model of the entire specimen. No assumptions of geometrical symmetry were prescribed.

The mesh consisted of approximately 3,000 second order hexagonal solid elements (C3D20R in ABAQUS™ [74]). Boundary conditions were applied at the upper and lower parts of the geometry, and tensile testing was simulated using a linearly increasing displacement. The simulations were performed using the ABAQUS™ implicit solver and the von Mises yield criterion.

Local variations in mechanical behaviour were incorporated using a layered approach, where physically measured values of SDAS at the top, middle, and bottom parts of the geometry served as input for the developed material characterisation models at these defined layers. In the intermediate layers, a linearly interpolated SDAS value was used. The developed computer program was applied to create the material definitions needed for the simulation.
CHAPTER 3

SUMMARY OF RESULTS AND DISCUSSION

CHAPTER INTRODUCTION

In this chapter, the main results in the supplementary papers are summarised and discussed. As has been previously mentioned, the papers address the stated research questions to various degrees.

3.1 EXISTING SIMULATION METHODS (SUPPLEMENT I)

During the literature review, three primary simulation approaches for cast aluminium components were identified. These methods are reviewed, compared and discussed in Supplement I. The methods can be briefly summarised as follows:

1. The Micro-structure based Mechanical Properties method (MMP) has been described above; briefly, however, it uses casting process simulations to predict local microstructure-based mechanical behaviour, which can be used as input for the FEM simulation.

2. The Fracture Criteria method (FC) uses a homogeneous material description and a fracture criteria to determine when fracture occurs in thin-walled HPDC components [76-79].

3. The Cradle-To-Grave method (CTG) uses a stress-state dependent damage evolution model to extend the functionality of a homogeneous material description in order to predict damage throughout a component [80-82].

In Figure 8, the various applications of the different approaches are presented schematically. The methods have, of course, been developed for different purposes, and thus have differing applicability. The MMP method predicts component-specific local mechanical behaviour for a wide range of alloys, and aims to use the results in FEM simulations. However, no method for the incorporation of local material behaviour into FEM simulations has been presented, and only examples which use homogeneous material behaviour have been reported [6]. The FC method uses data obtained from material and component testing to simulate fracture, but its applicability is limited to thin-walled components. The CTG method uses a damage evolution model that takes into consideration the effect of microstructural features,
such as Si particles and structural integrity, on the behaviour of the component. However, the method uses a large quantity of alloy-specific parameters, which need to be determined through extensive material testing, and thus its applicability is limited. To summarise, the MMP method generates material data, while both the FC and CTG methods are dependent on experimental material data and use FEM solver-specific extensions.

The literature review revealed the existence of different methods for considering specific microstructural features, such as Si particles and porosity, in a structural analysis of the component. None of these, however, take into consideration the local variations in mechanical behaviour throughout a cast component which stem from conditions that occur during the casting process. The MMP is able to predict these local variations using casting process simulations, but no method for transferring the results into an FEM simulation has been established.

Figure 8: Illustration of the application of the reviewed simulation methods (Supplement I).

3.2 MATERIAL CHARACTERISATION (SUPPLEMENTS II, VII)

3.2.1 ADI (Supplement II)

The effect of austempering on the plastic behaviour of two ADI alloys was investigated by varying the austempering temperature and duration (see Table 1 and Table 2 in Section 2.3.1). This was then followed by microstructural analysis and tensile testing, in order to evaluate variations in the strain hardening exponent and the strength coefficient of the Hollomon equation (Eq. 3) as influenced by austempering time and temperature. Figure 9 shows the tensile curves obtained for alloy ADI-1, as-cast and austempered for 1 h at various temperatures. The austempering is seen to have a significant impact on the mechanical behaviour, and different combinations of austempering parameters lead to different levels of strength and ductility.
Figure 9: Tensile test curves of ADI-1 as-cast and austempered for 1 h at various temperatures.

Figure 10 shows the variation in the strain hardening exponent for different austempering temperatures. A low austempering temperature results in a large undercooling and a fine structure, whereby a high volume fraction of ferrite and a low volume fraction of austenite is obtained [83]. The ferrite thus dominates the strain hardening behaviour as a result of its body-centred cubic structure with a low number of slip planes, offering a lower ductility and strain hardening rate than austenite, which has a face-centred cubic structure [49]. Thus, the initial achievement is a rather low value for the strain hardening exponent. Increasing the austempering temperature leads to a coarser structure with fewer interface areas and weaker interactions between dislocations and carbon atoms, consequently decreasing the strain hardening exponent [83]. When the austempering temperature is further raised, the increasing volume fraction of austenite comes to dominate the plastic behaviour, and the strain hardening exponent increases. The combination of a low temperature and short duration for austempering could lead to large amounts of metastable austenite, which may transform into hard and brittle martensite when stressed [84]; thus, a high value for the strain hardening exponent is achieved. The strength coefficient initially decreases with increasing austempering temperature due to the matrix coarsening but, at an austempering temperature above 300°C, the strength coefficient reaches a plateau or increases only slightly, although YS and UTS is reported to decrease. This is explained by the concurrent increase in the strain hardening exponent, and puts emphasis on the fact that the strength coefficient must be evaluated in combination with the strain hardening exponent.
Figure 10: Strain hardening exponent versus austempering temperature for (a) ADI-1 and (b) ADI-2.

3.2.2 HPDC aluminium (Supplement VII)

The gradient solidified specimens were used to establish a relationship between microstructural coarseness and the parameters of the Hollomon equation. The obtained microstructures in each experimental series with constant furnace speed are shown in Figure 11, wherein it is immediately obvious that the different cooling rates affect not only the SDAS, but also the morphology of Si and Fe precipitates.

Figure 11: Microstructure obtained in the (a) SDAS10 (b) SDAS25 and (c) SDAS50 experimental series.

The tensile behaviour (Figure 12) is seen to have a clear relationship to SDAS. It was noted that an intermediate microstructure has a slightly higher hardening rate than a fine microstructure at low plastic strains, but, under higher loads, a fine microstructure has a higher hardening rate. This effect was attributed to a solution hardening effect caused by back diffusion of Mg during solidification, which has been previously observed and confirmed by WDS measurements of gradient solidified
material [85]. The parameters of the Hollomon equation were evaluated for the different SDAS series (Figure 13) and relationships in the form of

\[ n_H = A \times \ln(\text{SDAS}) + B \]  

(15)

\[ K_H = C \times \exp(D \times \text{SDAS}) \]  

(16)

were found to provide a good fit to the experimental data, and are indicated by dashed lines in Figure 13.

Figure 12: Tensile curves obtained for the different experimental series of the HPDC alloy.

Figure 13: The relationship between SDAS-value and (a) strain hardening exponent and (b) strength coefficient. The curves depict the relationship predicted by the characterisation models (Eqs. 15-16).
3.3 SIMULATION STRATEGY DEVELOPMENT (SUPPLEMENT III)

3.3.1 Development and implementation

As revealed by the literature review (see Section 3.1 and Supplement I), there is no widely established method for transferring the local variations in mechanical behaviour predicted by a casting process simulation into a FEM simulation; in Supplement III, however, this topic was addressed by developing a computer program which incorporates the predicted local mechanical behaviour into simulation software. For the characterisation of material behaviour, the previously described method for predicting microstructure-based material behaviour was used (see Section 1.2.4).

The program creates FEM material definitions based on material behaviour parameters (i.e. $E$, $n_H$, $K_H$, $n_L$ and $k_L$, respectively), predicted by the casting process simulation for every element of the FEM mesh. A FEM material model described by a linear elastic and a piecewise linear plastic behaviour is used. This material model is available in most commercially available FEM solvers, and its use on the component level in FEM simulations is well established. As regards the current simulation strategy, however, the material model is applied on an element level throughout the component, meaning that one material description is defined for each individual element of the FEM mesh of the component. Alternatively, the program can group together elements with similar material parameter values and create a single material definition for each group. This is referred to as a material reduction technique.

The use of a piecewise linear plastic model implies that the non-linear curve described by the Hollomon or Ludwigson equations is specified at a user-defined Number of Linearisation Points (NLP) and, in the FEM simulation, the plastic behaviour is then linearly interpolated between these specified points. In order to obtain a more accurate description of the initial part of the stress-strain curve with high curvature, an interval divider approach was implemented, wherein the total plastic strain range is divided into two sections by an interval divider, leaving one half of the NLP within the first interval and the other within the second. This approach is schematically illustrated in Figure 14, where four NLP and an interval divider at $\varepsilon_{\text{div}}$ are shown. Although it is possible to develop more advanced methods for the efficient positioning of linearisation points, this method was selected as it provided an initial approach with the advantage of being easily implemented.
3.3.2 Software evaluation and verification

The piecewise linear plastic and interval divider approaches were evaluated using two Hollomon curves as reference points, with \( n_H \) values of 0.1 and 0.2. The mean percentage error of the linearisation was determined, and the interval divider approach was found to efficiently reduce the error of the linearisation without increasing the NLP. The performance of the developed software was evaluated for FEM models containing up to 500,000 elements. The time required for the software to generate all necessary material definitions and the file size of the FEM input file was measured, using both element-specific material definitions and the material reduction method. In addition, the differences between using the Hollomon and the Ludwigson equations at 20 and 40 NLP, respectively, were evaluated. It was found that, in the case of element-specific material definitions, both calculation time (Figure 15a) and FEM input file size increase linearly with the number of elements; the material reduction technique, however, was found to significantly reduce both calculation time (Figure 15b) and FEM input file size, particularly for a large quantity of elements. Increasing the NLP from 20 to 40 increases calculation time somewhat, and doubles the file size. The use of the Ludwigson rather than the Hollomon equation increases the calculation time slightly. It is also noted in Figure 15b that, when working with 500,000 elements in total, the calculation time for 100 material definitions is longer than for 1,000 material definitions. This is a result of the implementation of the program, and the handling of data in the random access memory and on the hard drive during the calculation, respectively.

**Figure 14: Schematic illustration of the linearisation of a Hollomon curve, using four linearisation points and an interval divider at \( \varepsilon_{\text{div}} \).**
Figure 15: Effect of the number of elements on software calculation time using (a) element-specific material definitions and (b) a reduced quantity of material definitions. H and L indicate which equation has been used, where H stands for the Hollomon equation and L for the Ludwigson equation.

The functionality of the software was verified by simulating a ductile iron engine support. A casting process simulation for the component was performed, including mould filling, solidification, and predictions of both the local mechanical behaviour and residual stresses. In Figure 16a, the predicted variations in the strain hardening exponent are shown. A FEM mesh of the component was created, and the developed computer program was used to create the material definitions needed for the FEM simulation, which was successfully performed in ABAQUS™ [74] (see Figure 16b).

Figure 16: (a) Variations in the strain hardening exponent $n_H$ (-) throughout the component, as predicted by the casting process simulation. (b) von Mises stress (MPa) obtained from a FEM simulation, where both local mechanical behaviour and residual stresses are included.
3.3.3 **Strategy formulation**

The computer program which was developed enables the use of the previously discussed MMP method as a basis for performing integrated simulations of cast components. This was formulated as a simulation strategy and designated *a closed chain of simulations for cast components*, schematically illustrated in Figure 17. The use of the word 'strategy' implies that it was not considered to constitute a verified and evaluated method, but rather a plan for achieving the integration of the casting process and FEM simulations. The nomenclature 'closed chain' implies the use of several different numerical models and simulations, as well as the transfer of all necessary data along each and every link of the chain. Additional links, e.g. machining simulations and optimisation methods, can also be added to the chain in future work.

![Figure 17: The closed chain of simulations for cast components.](image)

3.4 **SIMULATION STRATEGY APPLICATION (SUPPLEMENTS IV-VI,VIII)**

In order to investigate the relevance of the proposed simulation strategy for different materials, the effects of local variations in mechanical behaviour on the results of FEM simulations have been evaluated for both a ductile iron engine support and a HPDC aluminium flywheel housing.

**3.4.1 Local effects in ductile iron (Supplements IV-V)**

Several FEM simulations of the previously discussed ductile iron engine support were performed using different material descriptions and identical boundary conditions. A linearly increasing load, from 0 to 150 kN, was applied to the component. This load level was chosen to ensure that the maximum von Mises stress in the component would reach the approximate ultimate stress of the material during the last timestep of the simulation. In Supplement IV, only the errors for maximum stress and strain values (Max Value Error, MVE) were evaluated. In Supplement V, the investigation was broadened to include the distribution of stress and strain by selecting 10 gauge elements in the component and studying the locations of the maximum stress and strain values.
3.4.1.1 Local mechanical behaviour versus homogeneous behaviour

An investigation into the numerical differences between local mechanical behaviour and a homogeneous material description, as presented in the results of FEM simulations, was performed. A simulation with element-specific material descriptions and 60 NLP was used as a reference and designated LOCAL, and a homogeneous material description, based on the arithmetic mean values of each predicted material behaviour parameter throughout the component, was specified in order to isolate the effect of the variations in mechanical behaviour; this was referred to as AVERAGE.

The results show that a homogenous description of the material behaviour fails to account for the stress-strain response of the ductile iron component. In comparing the LOCAL and AVERAGE results, it may be seen that the local variations in mechanical behaviour cause a redistribution of stresses and strains throughout the component (Figure 18). This effect contributes in a critical way to the static behaviour and performance of the component.

![Figure 18: Comparison between predicted stress distribution by the (a) LOCAL and (b) AVERAGE simulation, at a load of 75 kN.](image)

This was numerically investigated, together with the effect of different NLP values and quantities of material definitions. Figure 19 shows that, although the predicted maximum von Mises stress value at all load levels is generally accurate, with an error of less than 5%, the predicted maximum von Mises strain value is far less consistent and has an error approaching 20% at high load levels. Moreover, and as illustrated above in Figure 18, the maximum stresses and strains are however predicted in incorrect locations. An increased NLP does not increase the accuracy of the simulation, because the assumption of homogeneous material performance itself is incorrect.
Figure 19: Relative error for (a) maximum stress and (b) maximum strain, using a homogeneous material description and varying quantities of linearisation points. The dashed line indicates where the 0.2% offset yield stress is initially exceeded.

The average errors in the von Mises stress and von Mises strain values for the gauge elements (Average Gauge Error, AGE) are low when the maximum stress is in the elastic region (see Figure 20), indicating that the prediction for stress-strain distribution is fairly accurate. However, there is an increase in errors when plasticity begins in the component, and the redistribution of load due to local mechanical behaviour is significant. It was found that the homogeneous description only predicts the correct location of maximum stresses and strains at low elastic loads and, in order to correctly predict the effect on the cast component at all load levels, the local variations in mechanical behaviour must be considered in the FEM simulation. If homogeneous material behaviour is assumed, the FEM simulation may thus lead to incorrect predictions of the behaviour and performance of the component. This supports the usage of the proposed simulation strategy, and the importance of considering microstructure-based mechanical behaviour in FEM simulations and during the development of cast components.
3.4.1.2 Local mechanical behaviour versus residual stresses

In Supplement IV, similar simulations to those discussed above were performed to study the separate contributions from the local variations in mechanical behaviour and the residual stresses to the overall component behaviour, utilising a reference simulation (LOCAL-RS) including both local mechanical behaviour and residual stresses. The results from the simulations which used only local mechanical behaviour (LOCAL), homogeneous mechanical behaviour (AVERAGE), or homogeneous mechanical behaviour and residual stresses (AVERAGE-RS), were evaluated as has been previously described. Simulations with homogeneous tabulated material data (TABLE, TABLE-RS) and a simple mean of the predicted maximum and minimum values of the material behaviour parameters (MAXMIN, MAXMIN-RS) were also included for illustrative purposes.

The results demonstrate that the residual stresses contribute significantly to the predicted stress level in the component at low elastic loads (see Figure 21). Under higher elastic loads, however, the effect of the residual stresses diminishes, and instead the accuracy of the results is determined by the type of material description. To correctly predict the behaviour of a cast component at all load levels, it is thus important to consider both residual stresses and local mechanical behaviour. The use of tabulated data or simple mean values leads to a high degree of error in the simulations.
3.4.1.3 **The effect of material reduction**

The investigation into the effect of material reduction was carried out by applying the technique so as to reduce the number of material definitions used in the component to between 30 and 12,000. The obtained errors for maximum stress and strain are shown in Figure 22, and the average gauge element errors are shown in Figure 23.

![Figure 21: Relative error in (a) maximum stress and (b) maximum strain, with and without consideration of residual stresses.](image)

![Figure 22: Error in maximum values of (a) stress and (b) strain, using local mechanical behaviour and material reduction.](image)

Figure 22 shows a fluctuating value for error in maximum stress and maximum strain when using a low number of material definitions, indicating that the
distribution of stresses and strains is not very accurately resolved. In Figure 22 and Figure 23, it is seen that, when using approximately 1,000 material definitions or more, the level of errors at any load is less than 0.25%, which is considered to be negligible. The FEM simulation time was found to increase by a factor of 2.5 when using element-specific material definitions rather than a homogenous one. Using material reduction lowered this factor to between 1.1 and 1.4, depending on the number of material definitions. If FEM simulation time is an issue, the material reduction method is thus an effective way of incorporating local variations in mechanical behaviour, without significantly increasing FEM simulation time or introducing any significant error into the FEM simulation.

![Figure 23: Average error in values of (a) stress and (b) strain in the gauge elements using local mechanical behaviour and material reduction.](image)

### 3.4.2 Local effects in cast aluminium (Supplements VI-VIII)

Similar numerical investigations as for ductile iron were performed for cast aluminium. In Supplement VIII, the same FEM model of the engine support that was used for ductile iron (Supplements IV-V) was investigated. This was undertaken in order to study both the difference between ductile iron and cast aluminium, and the effects of different solidification conditions, all while maintaining an identical geometry and FEM setup. The components were, however, not possible to produce as physical aluminium components.

In Supplement VI, the HPDC aluminium flywheel housing component was used. As a result of the fact that it was possible to produce these as physical components, physical verifications of the simulation results could be made. As seen in Figure 12, aluminium does not exhibit the variation in Young's modulus and elastic behaviour as seen in ductile iron; thus, its elastic behaviour is homogeneous, but variations in plastic behaviour can be seen before the 0.2 % offset yield stress. The Young’s modulus predicted by the casting process simulation for the flywheel housing is also homogeneous, but the local values of the parameters of the Hollomon equation are predicted by the previously described material characterisation models, (Eqs. 9-10).
These variations were incorporated into a FEM simulation with element-specific material definitions, here denoted LOCAL. As was the case for ductile iron, a homogenised material definition was also created, and referred to as HOMOGENISED. The load case was defined by adding surrounding parts using point masses and geometrical boundary conditions, and a gravity load which linearly increased from 0 g up to 25 g (where \( g = 9.82 \text{ m/s}^2 \) is the gravitational acceleration) was applied in increments of 2.5 g at every timestep. This load level was selected in order to obtain stresses in the range of the ultimate tensile strength of the material in the component. Similar to the ductile iron case, 10 gauge elements were selected, and the obtained variations of Max-Value Error (MVE) and Average Gauge-element Error (AGE) were determined.

### 3.4.2.1 Local mechanical behaviour versus homogeneous behaviour

The results show that cast aluminium display less local variations in mechanical behaviour than ductile iron. The impact of these variations on the overall distribution of stress and strain throughout the component is thus also lower. The local behaviour of highly stressed regions at high loads is, however, affected; see Figure 24, where Figure 24b presents the difference in stress levels predicted by the LOCAL and HOMOGENISED simulations. This indicates that the effect on static stress and strain redistribution is numerically smaller in HPDC aluminium than in ductile iron, but not insignificant. This conclusion is supported by the results for the engine support which was examined in Supplement VIII. The variations in behaviour were here noted to cause a redistribution of the location of maximum stress and strain, as previously described for the ductile iron case. In Supplement VIII, the effects of different solidification conditions on the distribution of local variations in mechanical behaviour, and on component behaviour, were also highlighted.

The achieved variations in MVE and AGE in the flywheel housing simulations are shown in Figure 25. A similar behaviour as in the ductile iron case is noted, where the effect of the local variations in behaviour rises with increased load. Even prior to the 0.2% yield stress being reached (indicated by the dotted line), a numerical error in MVE is seen, and is explained by variations in non-linear behaviour that occur even under very small plastic loads. As the load level increases, so too do the errors, which reach a maximum of 2.5% in stress level and 1% in strain. Comparing the results for HPDC aluminium (Figure 25) and sand cast ductile iron (Figure 19 and Figure 20), the obtained level of errors is significantly lower in the case of the former than the latter, where errors up to 20% occurred. The variations in mechanical behaviour are smaller, and thus the effect of the variations is also reduced in aluminium when compared to ductile iron.
Figure 24: (a) Stress distribution as predicted by the LOCAL simulation at a load level of 15 times gravitational acceleration. (b) Difference between the LOCAL and HOMOGENISED simulation stress levels at a load of 15 times gravitational acceleration.

Figure 25: The effect of local variations in material behaviour of the HPDC aluminium component at different load levels, measured in multiples of gravitational acceleration. (a) Relative error in maximum stress and strain. (b) Average error in stress and strain in the gauge elements. The dashed line indicates where the tabulated 0.2% offset yield stress is initially exceeded.

3.4.2.2 Local mechanical behaviour versus residual stresses

The HPDC process is known to cause high residual stresses, and, for the current component and casting process, values of up to 150 MPa are predicted in the component by the casting process simulation. As for the ductile iron case, the separate contributions from local variations in mechanical behaviour and residual stresses can be studied for the aluminium case. Thus, one FEM simulation including local mechanical behaviour and residual stresses (LOCAL+RS) and one FEM
simulation using homogenised behaviour and residual stresses (HOM.+RS) were added to the evaluation. The obtained variations in MVE and AGE, where LOCAL+RS is the reference simulation, are shown in Figure 26. It is seen that the residual stresses contribute greatly at small loads, while the effects of the variations in mechanical behaviour are very small. As the load increases, however, the effects of the residual stresses diminish, and the effect of local variations in behaviour increases. This shows that both residual stresses and local variations in mechanical behaviour should be incorporated into the simulation in order to accurately predict the behaviour at all loads.

![Figure 26: The numerical effect of the local variations in material behaviour and residual stresses. (a) Relative error in maximum stress and strain. (b) Average error in stress and strain in the gauge elements. The vertical dotted line at 7.5 g indicates where the tabulated 0.2% offset yield stress is first exceeded.](image)

### 3.5 SIMULATION STRATEGY VERIFICATION (SUPPLEMENTS VI-VII)

The accuracy of a simplified casting process simulation, which was used to predict variations in microstructural coarseness throughout the HPDC aluminium flywheel housing, was studied by investigating the microstructural coarseness in 10 different locations throughout the component. Comparisons to simulated values generally showed a strong agreement, with some deviations due to the simplifications applied in the simulation.

Tensile testing of samples from different areas of the component confirms that material behaviour is not homogeneous throughout (Figure 27). The simulation strategy was found to accurately predict the distribution of these variations; it was noted, however, that the simulation generally predicted a slightly higher value for strain hardening than was achieved in the component, particularly in coarser microstructures (Figure 27). This was attributed to the fact that the implemented models have been developed for sand cast alloys containing up to 0.65% Fe, while the investigated HPDC alloy contained 0.8% Fe, thus increasing the likelihood of the formation of detrimental iron-rich intermetallics. This provided an impetus for the previously discussed material characterisation study for this alloy (see Section 3.2.2).
Figure 27: Measured variations in mechanical behaviour in the HPDC component, and a comparison of simulated and measured tensile behaviour of a region containing a fine (SDAS 6-8 μm) and a coarser (SDAS 14-16 μm) microstructure in the HPDC aluminium component.

The developed material characterisation models (Eqs. 15-16) were implemented into the tensile testing FEM simulation of the experimental series, with gradual variations in microstructural coarseness. A simulation which incorporated considerations of local variations in microstructure, LOCAL, was performed, as well as a simulation based on the assumption of homogeneous material behaviour, HOMOGENEOUS, which used the intermediate SDAS value in the specimen as input for the characterisation models.

The simulated strain distributions were compared to those observed using DIC. It was seen that the strain level at low plastic loads (Figure 28) was somewhat greater in the upper part of the specimen (SDAS 10 μm) than in the lower section, where the microstructure is coarser (SDAS 20 μm). This was attributed to the previously described solution hardening effect, which causes a higher hardening rate in the lower part than in the upper, meaning that a higher strain is obtained in the latter section. As the load level increased (Figure 29), the distribution of strain shifted, and the highest strain level instead occurred in the lower part of the specimen.

This behaviour was correctly predicted by the LOCAL simulation. The HOMOGENEOUS simulation, however, failed to predict the correct location of maximum strain, as the assumption of continuously homogeneous material behaviour led to the predicted strain distribution being symmetrical; i.e. it was predicted that both the upper and lower parts of the specimen would be subjected to the highest strain at all loads. This level of variation in microstructural coarseness can be considered to be representative of the microstructural variation found in cast aluminium components, and so these results may thus be considered to be representative of the actual behaviour within components. They also verify the applicability of the proposed simulation strategy, and demonstrate the importance of correctly describing the local variations in mechanical behaviour in order to correctly predict the strain distribution throughout cast components.
Figure 28: Strain fields observed using DIC and predicted by the LOCAL and HOMOGENEOUS simulations, at a load of approximately 180 MPa.

Figure 29: Comparison between strain fields observed using DIC and predicted by the LOCAL and HOMOGENEOUS simulations, at a load of approximately 300 MPa.
CHAPTER 4

CONCLUDING REMARKS

CHAPTER INTRODUCTION

This chapter summarises the work carried out in this thesis and some of the conclusions that have been arrived at.

A new simulation strategy, referred to as a closed chain of simulations for cast components, has been developed. The simulation strategy enables the use of predicted local mechanical material behaviour in the product realisation process for cast components. The strategy has been shown to be both relevant and accurate, and has been verified by physical experiments.

The development of the strategy has been performed in four main steps:

1. Literature review and comparison between existing simulation methods.
2. Strategy formulation and implementation.
3. Numerical experiments and investigations.
4. Validation using physical experiments and material characterisation.

The effects of local variations in mechanical behaviour on the overall behaviour of cast components have been established. Numerical experiments for both ductile iron and aluminium components have shown the relevance of the strategy, and physical experiments have been performed to verify the simulation results.

Digital Image Correlation has been used to physically observe the numerically predicted redistribution of strains caused by local variations in microstructure. This was accurately predicted by simulations using local material behaviour.

The work has successfully laid the foundations for an increased use of casting process modelling by integrating casting simulations into the design process for cast components. This facilitates an improved fit of the product development/production interface, and new possibilities for the design of industrial cast components with high performance.
CHAPTER 5

FUTURE WORK

CHAPTER INTRODUCTION
In this chapter, ideas are presented on how to improve and verify different parts of the simulation strategy in future work.

5.1 SIMULATION
The simulation strategy offers a chain of simulations, from casting process to component behaviour, that provides an opportunity to study the effects of different materials and casting process variations, not only for microstructure formation and residual stresses but also as concerns the mechanical performance of a component. Further studies in this area may concern e.g. the screening of important material and casting process variables, process optimisation, or product robustness analyses.

Only static behaviours have been studied in the current work. It is, however, reasonable to claim that variations in microstructure and material behaviour have a significant impact on the dynamic and fatigue behaviour of components. Further studies in these areas are suggested.

Although the elasto-plastic behaviour is shown to be well described, there are currently no considerations of damage or failure implemented into the structural analysis. The current simulation strategy provides a new way of determining the stress-strain distribution throughout a component, which can be used as an input for simulations of fracture behaviour. Further work in this field may include extending the simulation strategy to involve fracture mechanics based on simulations of crack propagation and component failure.

The numerically predicted strain redistribution, which is due to local variations in microstructure, has been confirmed using 2D DIC on gradient solidified flat tensile specimens. Future works which extend this approach to Stereo DIC of 3D geometries on real components would provide further confirmation of the simulation strategy, and lead to an improved understanding of the effect of local material behaviour on component behaviour.

5.2 MATERIAL CHARACTERISATION
The simulation strategy is highly dependent on the quality of the material characterisation used in the casting process simulation, and the error introduced by
the microstructural characterisation is likely to be more significant than the errors due to the linearisation or material reduction processes that have been investigated in this thesis. It is thus essential that the characterisation models used are further verified and improved. In addition, the discussed models have been developed for as-cast materials and specific ranges of alloying elements; thus, the characterisation models need to be extended to include the effects of heat treatment and a greater range of alloys.

Several microstructural features, which affect mechanical behaviour to varying degrees, are still not included in the simulation strategy; these include defects, oxide films, and several alloying elements. To improve the overall accuracy of the simulation strategy, these effects should be further studied and incorporated.

The effect of austempering on the plastic behaviour of ADI has been investigated. In order to be able to include ADI in the proposed simulation strategy, however, numerical models for microstructure transformation during austempering, and the relationships between microstructure and mechanical behaviour, need to be established.
REFERENCES

## APPENDED PAPERS

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