Simulation of Welding and Heat Treatment

Modelling and Validation

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Abstract

Many aerospace components with complex geometry are fabricated from smaller parts using joining techniques such as welding. Welding and the heat treatment which usually follows, can result in unwanted deformation and stresses. Expensive materials, tight geometrical tolerances and the need to decrease product and manufacturing development time, cost and associated risks have motivated the development of models and methods for the simulation of manufacturing processes.

The work presented concerns methodologies and modelling techniques for the simulation of welding and heat treatment of fabricated aircraft-engine components. The aim of the work was to develop modelling practices to enable the use of finite element analysis for the prediction of deformation, residual stresses and material properties such as microstructure during and after welding and heat treatment. Achieving this aim has required investigation of geometrical discretisation, modelling of boundary conditions and material behaviour for these processes. The case study components were made of a martensitic stainless steel, Greek Ascoloy. Phase evolutions models and models for rate-independent, rate-dependent, and creep were used as the material models in the welding and heat treatment simulations. The work also includes discussion of numerical considerations in material modelling. A toolbox for evaluation of constitutive models and to obtain material parameters for the plasticity models was developed. The heat transfer coefficient is an important parameter for describing energy transfer between the component and a gas. Due to the complexity of the gas flow in the heat treatment furnace during cooling, a method using computational fluid dynamics was developed to obtain an approximate distribution of the heat transfer coefficient.

Due to the impact that modelling and simulation predictions can have, the creditability of the computational results are of great concern to engineering designers, managers and other affected by decisions based on these predictions. In this work, a validation methodology for welding and post weld heat treatment models was developed.

The model used for welding simulations gives results with the accuracy required for predicting deformation and residual stresses at all stages of the product and manufacturing development process. The heat treatment model predicts deformations and residual stresses resulting from stress relief heat treatment of sufficient accuracy to be used in the concept and preliminary stages of product and manufacturing development. The models and methodology have been implemented, tested and are in use at Volvo Aero.

Keywords: Computational welding mechanics, heat treatment fluid-structure interaction, plasticity, finite element method, residual stresses, validation
Appended Papers

This thesis is based on the work contained in the papers listed below:

**Paper I**
Simulation of Welding and Stress Relief Heat Treatment of an Aero Engine Component
Daniel Berglund, Henrik Alberg, and Henrik Runnemalm

**Paper II**
Constitutive modelling and parameter optimisation
Lars-Erik Lindgren, Henrik Alberg, and Konstantin Domkin
Proceedings of the 7th International Conference on Computational Plasticity – COMPLAS 2003, Barcelona, Spain, 7 - 10 April 2003

**Paper III**
Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment
Henrik Alberg and Daniel Berglund

Corrigendum to: "Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment"
Henrik Alberg and Daniel Berglund

**Paper IV**
Comparison of an axisymmetric and a three-dimensional model for welding and stress relief heat treatment
Henrik Alberg and Daniel Berglund
Proceedings of the 8th International Conference on Numerical Methods in Industrial Forming Processes – NUMIFORM 2004, Columbus, OH, USA, 13-17 June 2004

**Paper V**
A two stage approach for validation of welding and heat treatment models used in product development
Daniel Berglund and Henrik Alberg
Science and Technology of Welding and Joining, Volume 10, Issue 6, pp. 653-665
Contributions to Co-authored Papers

Five papers and one corrigendum are appended to the thesis. All the papers have been written in collaboration with co-authors. The work carried out in each paper has been jointly planned by the authors.

Paper I
The author carried out the modelling and simulation of the heat treatment process.
The author wrote part of the paper.

Paper II
The author carried out the material parameter identification.
The author wrote part of the paper.

Paper III
The author implemented the constitutive models.
The author carried out major part of the heat treatment simulations.
The author carried out part of the welding simulations.
The author wrote major part of the paper.

Corrigendum to Paper III
The author carried out the welding and heat treatment simulations as presented in the original paper. The author found, and submitted the corrigendum for the error concerning the dilatation model, where the transformation strain for the austenite to martensite transformation was accidentally put to zero.

Paper IV
The author carried out major part of the modelling.
The author carried out the welding and heat treatment simulations.
The author wrote the complete paper.

Paper V
The author implemented material models for plane stress condition; rate-independent plasticity including TRIP and creep model.
The author carried out part of the welding simulations.
The author wrote part of the paper.
Preface

This work has been carried out at the Division of Computer Aided Design (CAD) at Luleå University of Technology (LTU), during the period 2000-2005, with a six months’ leave of absence. The work was supervised by Professor Lars-Erik Lindgren at LTU and Dr. Henrik Runnemalm at Volvo Aero.

I would like to express my gratitude to Professor Lindgren for his support, discussions and critical review of my work, and for his great enthusiasm. Also thanks to Dr. Henrik Runnemalm at Volvo Aero who made it possible for me to work in Trollhättan and for the discussions and advice. To Dr. Daniel Berglund my friend, colleague, and co-author of several papers. Thank you Daniel for encouragement, advice and numerous discussions about work, nuclear power and other fascinating issues and not least, thanks for all the laughs!

I would like to thank, the Head of the Division of Computer Aided Design, Professor Lennart Karlsson, his staff and all my colleagues at the division. You have made my stay in Luleå most pleasant. I would like to express particular gratitude to Andreas Lundbäck for being a good travel and discussion partner during my work and to Markus and Simon Lindgren for their work doing the residual stress measurement during two summer vacations. My daily work has been carried out at the Division of Advanced Material and Manufacturing Technology at Volvo Aero in Trollhättan. I would like to thank my colleagues, former and present, at the division for the excellent working environment and for sharing their knowledge in many different areas.

I would finally like to thank my family and friends – my parents and my sister for always supporting and believing and in me during my struggles. My friend Viktoria for all her encouragement and for being there. I express my gratitude to Siw and Kjell Rönneqvist for letting me live your in house during my stays in Luleå. You have made these stays very pleasant.

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Henrik Alberg
Trollhättan, September 2005
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Review and Summary of Thesis

1 Introduction

Doing things right the first time is essential when developing products and manufacturing processes in the industry. Using manufacturing simulations makes it possible to evaluate several alternatives before a product or prototype exists. Using manufacturing simulations properly can shorten product and manufacturing development time, reduce cost, minimise the need for testing and at the same time improve quality. This work presents a methodology and models for the simulation of welding and heat treatment processes to be used in the development of aerospace components and their manufacturing processes.

1.1 Background and motivation for the study

Many aircraft-engine components are manufactured from single castings or fabrications and usually have a complex shape. Typical the parts have a diameter of one meter or more and are usually made of high-strength, corrosion and creep resistant materials such as titanium alloys (e.g. Ti-6Al-4V and Ti-6Al-2Mo-4Zr-2Sn), nickel-based alloys (e.g. Alloy 718) and martensitic stainless steels (e.g. Greek Ascoloy). In a single casting, the main structure of the component is cast and only minor parts such as flanges are attached to the casting. Due to relatively large the diameters of the components and the materials use, the number of foundries capable of producing such castings is limited.

With fabricated components, several castings, forgings or formed sheets, are joined together to produce the final component. The individual parts are often joined together by welding, which is usually followed by heat treatment. There are generally more subcontractors capable of manufacturing these smaller items. Fabrications offer several advantages. Most added value, and hence profit, lies with the assembler and not with the foundry. Another advantage over single castings is that it is possible to choose different materials for different parts of the component. However, fabrication involves a large number of operations and relatively complex processes such as welding and heat treatment, which are susceptible to problems such as deformation and the formation of residual stresses. Over the years, craftsmen have increased their skills and knowledge in order to minimise problems associated with fabrication. These skills have generally been acquired either by trial and error or by using a more systematic problem solving approach.
Aerospace components, with their expensive material, narrow geometrical tolerances, coupled with increasing demands to reduce product and manufacturing development time as well as the risks and costs associated with large industrial projects has lead to an increasing need to do things 'right first time.' This in turn has lead to the development of modelling and simulation techniques, which can reliably predict the effect of manufacturing processes such as heat treatment on a component. Decreasing costs, time, and risk by increasing the information available about a product and its manufacturing processes will help a company achieve a better market position and improve competitiveness.

1.2 Aim, scope and approach of the current work

The aim of this work was to establish a modelling and simulation methodology that enabled the prediction of residual stresses, deformation and material properties such as microstructure (phase content) during and after welding and heat treatment. The results of the simulations had to be sufficiently accurate and completed within an acceptable time frame to allow them to be used in product and manufacturing development.

The problem required different levels of geometrical discretisation and modelling of boundary condition and material behaviour for the processes investigated. Given that manufacturing is a sequence of several processes, it was important to cover simulation of as many processes as possible. This will also allow optimisation of the entire manufacturing chain instead of optimising each individual process, which could give sub-optimal results. Due to the consequences that modelling and simulation prediction can have, the credibility of the results is of great concern to engineering designers, managers, and other affected by decisions that are based upon these predictions. Therefore, strategies for validation and qualification of simulation models are very important. Given the discussion above the following research question was formulated,

*How should modelling and validation of welding and heat treatment be carried out in order to provide adequate accuracy to support product and manufacturing development?*

The research presented in this thesis is limited to thermo-mechanical models of single pass fusion arc/beam welding and does not including welding related phenomena such as weld pool geometry, nor microstructural developments such as grain evolution or grain boundary liquation. The heat treatment process investigated was limited to stress relief in gas-cooled vacuum furnaces. The material of interest throughout this work was a martensitic stainless steel, Greek Ascoloy. The Finite Element Method (FEM) was used for solving the partial differential equations governing heat transfer.
and structural behaviour. Additionally, a finite volume method was used to solve the partial differential equations governing gas flow in the heat treatment furnace.

Commercial finite element software was used as the base of the simulation model which was implemented as user subroutines linked to the commercial FE code. A deductive approached to the research was used. Known technologies were tested and the limitations of the models and techniques developed are investigated when used in welding and heat treatment applications. The work was carried out in cooperation with the Swedish aerospace industry and the results used and evaluated in demonstrators and in industrial product development projects.

1.3 Definition

Some terms are misused or may have different meanings in different research fields. To avoid ambiguousness, the usage of the following terms are defined:

- **Model:** A symbolic device (here a finite element model and related information) built to represent certain aspects of reality.

- **Modelling:** The breakdown, simplification etc. of a process in order to create a model.

- **Simulation:** The actual computation using all the models implemented in the software.

- **Simulation tool:** The apparatus (pre-processor, post-processors, solvers, etc.) used to carry out the simulation.

- **Adequate accuracy:** The required level of accuracy needed at a given point in time to give a satisfactory answer to the questions addressed by the simulation.

- **Validation:** The process of determining the degree to which a model is an accurate representation of real world from the perspective of the intended uses of the model.

- **Verification:** The process of determining whether a model accurately represents the developer’s conceptual description of the process and that the solutions from the simulation accurately represent the actual process.

- **Qualification:** Determination of the adequacy of the conceptual model to provide an acceptable level of agreement for the domain of intended application.

The definition of validation and verification are based on the definition given by the American Institute of Aeronautics and Astronautics (AIAA), and that for qualification is based on the definition given by the Society for Computer Simulation (SCS)
all presented in Oberkampf (2002). Other definitions of validation, verification and qualification exist. Examples are presented in or referenced in Oberkampf (2002).

1.4 Structure of the thesis

This thesis consists of an introductory part and five appended papers. The introduction begins with a presentation of different welding and heat treatment processes. A discussion of the use of manufacturing simulations in product and manufacturing development follows with some examples. Techniques for material modelling including phase transformation and the governing constitutive equations are then presented. Methodologies to obtain material parameters are also considered and exemplified. Issues related to the modelling and simulation of welding and heat treatment are then discussed. This is followed by a validation strategy for a welding and post weld heat treatment models. Finally, conclusions, suggestions for further work and the scientific contribution made by the current work are given.

Papers I and III outline the current state of computational welding mechanics and heat treatment simulations and compares some constitutive models. A methodology for simulation of combined welding and heat treatment is also presented. Paper II presents methodologies and a tool to obtain material parameters. This is supported by a single case. Paper IV examines the influence of geometrical discretisation when doing simulation of combined welding and heat treatment on an aerospace component. Paper V concerns validation strategies and includes a strategy for validation of simulation of welding and heat treatment.

2 Welding and heat treatment of metals

The earliest examples of welding and heat treatment occurred in the Bronze Age in the Eastern Mediterranean. However, it was not until the 19th century that welding, as we know it today was invented. This was facilitated by the discovery of acetylene in the 1830’s and at about the same time the invention of the arc-welding process. In late 1800’s and early 1900’s, resistance welding and thermit welding were invented. The use of externally applied shielding gasses was widely researched in the 1920’s and resulted in the development of Gas Tungsten Arc Welding (GTAW) or Tungsten Inertia Gas (TIG) welding and Gas Metal Arc Welding (GMAW) in the 1940’s. These techniques used helium or argon for shielding. Several other welding techniques have been developed since then including electroslag welding, plasma arc welding, electron beam (EB) welding, friction welding, and laser welding.
This work concerns the fusion welding processes, in which the metal parts are heated until they melt together. Fusion welding can be carried out with or without the addition of filler material. A necessary part of this welding process is a source of heat sufficient to melt the material being joined (and any filler metals added). Arc welding, EB welding, and laser welding belong to this category of welding processes and are commonly used in the aerospace industry.

In TIG-welding, heat is produced by an electric arc between a non-consumable tungsten electrode and the workpiece. An inert gas, such as argon, is used to prevent oxidation of the weld zone and the electrode. Filler material can be used and the process is best suited for materials with a thickness of 0.5 to 3 mm. In EB-welding, a concentrated electron beam with a high power density is used to melt the material. The welding operation is carried out in a low-pressure environment to reduce the retardation of the electrons and to avoid oxidation of the weld zone. The fusion zone is smaller than for TIG-welding and the penetration depth is large. EB-welding has the advantage of giving small residual deformations and is well suited for butt-welding of thick material up to about 250 mm. In laser welding, a high energy density laser beam is used to melt the material. The advantage of laser welding compared to EB-welding is that the process does not require a low-pressure environment, however some protection to prevent oxidation in the weld zone is needed. Another advantage of laser welding is that the laser light can be transported from the laser source to the workpiece by mirrors or optical fibres. Common lasers types used for welding are CO\textsubscript{2} and Nd:YAG-lasers. Laser welding is most efficient for thin plate applications.

![Figure 1: An idealised heat treatment sequence.](image)

Heat treatment is a collection of many processes such as annealing, stress relief, quenching, tempering, and ageing each of which aims to change one or more material properties such as hardness, strength, toughness, and wear resistance. The basic principle of heat treatment is simply heating and cooling, Figure 1. This simple process can result in complex changes to the underlying microstructure of the materials. The
temperature and time required for the various processes depends on the mechanism controlling the required effect. For example, if the driving mechanism is diffusional, the heat treatment time must be sufficiently long to allow any necessary transformation reaction. During heating or cooling, temperature gradients develop in the material; their magnitudes depend on for example the size and geometry of the product. If the temperature gradients are large, then they can create stresses which may lead to plastic deformations or in the worst case, to cracking. Other phenomena that may induce unwanted deformations or cracking are microstructural changes such as martensitic transformations or strain-age cracking. It is therefore important to control any heat treatment process so that unwanted effects are avoided or minimised.

![Figure 2: Schematic diagram of a gas cooled vacuum furnace.](image)

The heat treatment process studied in the present work is carried out in a gas-cooled vacuum furnace (or simply vacuum furnace), Figure 2 which offers flexibility and is used for many types of heat treatment processes. Vacuum furnaces minimise or prevent surface reactions on the product such as oxidation or decarburisation. In the vacuum heat-treatment process examined here, the product is heated by thermal radiators in an evacuated heated enclosure at operating pressure of about 0.01%-0.1% of atmospheric. During the cooling sequence, gas is pumped into and through the charge volume from an external vessel, Figure 2. The inlet and outlet vents can usually be altered to obtain a more even cooling of the component. The cooling gas is recirculated until the component reaches the required temperature. The post weld heat treatment studied is carried out to reduce stresses in the component. Additional information on heat treatment processes and equipment can be found, for example, in the ASM Handbook on Heat Treating, Davis (1991).
3 Manufacturing simulation in industry

Manufacturing simulations are used when developing products and associated manufacturing processes either with new or existing products and also when considering investment in new equipment. Manufacturing simulations link design and manufacturing during product development and act as a tool for design and manufacturing engineers to evaluate different concepts or manufacturing processes. Runnemalm (1999) divided the design part of the product development process into three stages namely concept design, preliminary design, and detailed design and the manufacturing part of the product development process into three stages namely inventory of known methods, preliminary preparation, and detailed preparation, Figure 3. In Paper V, the scheme by Runnemalm is extended with a pre-development stage. This view of the design process is used as the basis of the discussion related to the aero engine industry presented in this chapter. The discussion is also reasonably generic and can be easily applied to many other manufacturing industries. In the subsequent sections the requirements, issues and cases where manufacturing simulations are used are examined.

![Figure 3: Key activities during the product and process development, after Runnemalm (1999).](image)

The methodology and models developed here can be used in all stages of product and manufacturing development. However, it is crucial that the methods and models used to carry out manufacturing simulation are developed and implemented in the product development process used by a company before the simulations need to be used in live development projects. During an ongoing product development project, there are no or little time for development, for acquiring material data and validation of the models to be carried out. If manufacturing simulations are not well developed, much time can be wasted since the model cannot be fully utilised. Development timescales are becoming shorter and shorter. For example, a current engine component development project in the aero-engine industry is planned to take only 15 months from the start of design to the first engine tests. With timescales like this, there are obviously
not much time for problem solving simulation models, acquiring new material or process data.

When developing manufacturing simulation models, several activities need to be completed; most importantly defining the specifications and requirements placed on the simulation model. Given these, the development phase can start and methods and models chosen. Material and other critical data must be acquired and verification, validation, and qualification of the simulations carried out. Finally, the models and methods can be implemented in the product development process.

### 3.1 Development of new products

In the concept design stage, manufacturing simulations are used to examine different design and manufacturing concepts such as location of welds on fabricated components. At this stage, a fast response is very important. This means that pre-processing (modelling activities: geometrical discretisation, applying initial and boundary condition, input of material data, and so on), analysis time, and post-processing (extracting results) must be as short as possible. The results from these simulations are used to answer broad questions with a simple yes or no and/or to choose between different design concepts. To reduce modelling and analysis time, two-dimensional models and material models that do not take into account complex interactions are usually preferred.

In the preliminary design stage, the location of welds, for example, can still be an important issue however changing these is best avoided since the design at this stage should be more or less fixed. From a manufacturing point of view, it is at this stage that any fixtures needed for welding and heat treatment are designed. Issues related to this include:

- How much will the component deform during welding, i.e. maximum, or minimum transient deformations?

- Where should the product be clamped and should springs be used to allow movement of the component in the fixture?

There are also other issues designing fixtures, not directly related to the current work; the size and weight of the fixture must allow it to fit into production equipment and the piping for directing shielding gas must be designed.
For preliminary design activities, three-dimensional models are usually used which increases the analysis time. The simulations may still used to identify tendencies and answer simple yes/no questions, especially with fixture design, but the product manufacturing simulations need to be of higher accuracy than at the earlier stage since the magnitude of stresses and deformations are of interest. A material model where relatively few effects are accounted for is still usually preferred since short analysis times are still required. From a manufacturing point of view, the detailed design stage concerns optimisation of welding and heat treatment sequences since only minor changes in the fixtures and product design are possible. At this stage, three-dimensional models using the finest possible discretisation are usually required and materials models including most or all of the physics, which can be handled by the simulation model, is preferred.

It is important to note that the heat treatment process is generally fixed from the start due to material requirements and equipment limitations. However, there are some heat treatment related issues that have to be solved. The required heating rates will dictate whether radiative, convective, or a mix of these be used for heating the product. If radiative heating is used, the question of the location of heating elements needs to be answered e.g., heating by a single element from one side or multiple elements. If convective heating is used, should natural or forced convection be used? During cooling, there is usually a requirement to achieve a certain cooling rate in order to create the desired microstructure. It is quite common that high cooling rates are required. It is also important to achieve even cooling of the product to avoid thermal gradients. To obtain the required cooling rates and even cooling management of the gas flow may be necessary. For example, thin areas of the product may have to be shielded from the gas flow to avoid to rapid cooling whilst thicker areas may require extra cooling.

In the earlier discussion, the heat treatment process may seem to be forgotten. However, deformations produced during welding are not the only deformations that occur since post welding heat treatment and even machining will result in deformations, which the manufacturing team should be aware of.

### 3.2 Further development of existing products

Manufacturing simulations can be used when developing existing manufacturing processes and facilities. This will include troubleshooting and changing manufacturing process plans. Workshop troubleshooting in this work relates to errors or problems with one or few products. Component design and manufacturing processes can be altered during the life of a product, due to cost reduction projects or to solve known problems. Questions related to these could be:
• What happens if the stress relief heat treatment is not carried out between manufacturing operation A and manufacturing operation B?

• A reduction in residual deformations and/or residual stresses is required. Can this be achieved if the welding is carried out in another sequence or using another method?

• The incoming material is to be changed from a casting to a forged material. How will this affect the stresses and deformations in the final product?

• The life of a product is currently 2000 cycles. New design requirements state that a life of 5000 cycles is required. How can manufacturing help achieve this?

In workshop troubleshooting projects, questions could include:

• The product suffers from cracks in the heat-affected zone. Can these be avoided if the weld location is moved and/or divided into smaller sections?

• Can the product be repaired by welding whilst still maintaining the necessary geometrical tolerances?

Workshop troubleshooting usually requires a fast response. However, it is difficult to give general advice as to which simulation and material model should be used due to the great variety and complexity of the questions that can arise.

### 3.3 Investment in new equipment

A manufacturing simulation tool can be of great help when new equipment is to be acquired. In this section, a case from Volvo Aero in Trollhättan is presented. This project concerned investment in a new heat treatment furnace. The workshop already had several furnaces of different size, thermal radiator design, and cooling design. Cooling design involves optimising the use of the gas inlets and outlets used during the cooling sequence. These are located in different places and are of different size and number in different furnaces. The task was to investigate how different cooling design, primarily the location of the inlet and outlet vents, affected the cooling rate in the component. The main question was "Which furnace design will fulfil the stated heat treatment requirements?" The methodology and models developed in this work (Paper A) could be used to help such investigations.
4 Material modelling

A critical issue in the development of a finite element model for manufacturing simulation is the material model used. This involves choosing a suitable material model, obtaining material data and key material parameters and developing a numerical implementation of the stress calculation algorithm. In the following sections, the modelling of phase evolution and constitutive models is discussed. In addition, a method to obtain material model parameters and numerical considerations in material modelling are given. This chapter describes how the chosen equations are used and treated. It is not intended to cover all the assumption made and physics behind the equations used to describe material behaviour.

4.1 Phase evolution models

Numerous microstructural phenomena such as weld solidification microstructures, evolution of phase transformations, or grain boundary liquation can be modelled and it is essential to include these into the material model when the microstructure and material properties change considerably. When modelling phase transformations two features must be examined, the models used for phase evolution and the assumptions made as to how and which material properties are affected by the different phases. Greek Ascoloy is a martensitic stainless steel that forms phases such as ferrite, pearlite, austenite, martensite, and bainite. Three different structures have been modelled. One is the mixture of ferrite and pearlite, which is considered as a single phase in the model. The other two phase structures are austenite and martensite. The phases evolve under different conditions where time, temperature, and relative amounts of different phases are important.

One way to measure and illustrate the effects of phase transformations in a material is to use a thermal dilatation test. In this test, a specimen is heated and subsequently cooled to the initial temperature. Throughout the test the strain, called thermal dilation $\varepsilon_{\text{dil}}$, is measured, Figure 4. From such test, several important observations can be made and parameters for the phase evolution models extracted. In Figure 4 four main sections can be identified; between I and II an increase in temperature results in an almost linear increase in thermal dilation. Between II and III, a increase in temperature produces a non-linear increase in thermal dilation due to the formation of austenite. Between III and IV, the material is cooled and a nearly linear relation between temperature and thermal dilatation is observed. Between IV and V, an abrupt change in the dilation is observed due to the formation of martensite. The goal is to accurately model thermal dilation behaviour since this is the principle coupling between the thermal and the mechanical domains. Thermal dilation is defined in Eq. (1) and where $\varepsilon^{th}$ is the volumetric thermal expansion and $\varepsilon^{\text{ra}}$ the volume changes due to
phase transformation. The idea behind modelling thermal dilatation is to first model the phase evolution, and then based on the state described by the phase evolution model, calculate the thermal dilatation.

\[ \varepsilon_{dil} = \varepsilon^{th} + \varepsilon^{tra} \]  

Two phase evolution models and associated calculation of the thermal dilatation have been investigated. In the first model, proposed in \textit{Paper I}, phase evolution is controlled by the peak temperature as follows. Austenite transformation is assumed to occur if the temperature experienced by the material is greater than that of the end of austenite transformation temperature, \( A_{e3} \), Figure 4. The martensite transformation is assumed to occur if the temperature experienced by the material is below the end of the martensitic transformation temperature, \( M_e \), Figure 4, and only for austenitic material consisting, since martensite forms from austenite and not from ferrite or pearlite. In this model, a material can only consist of a single phase at any one time, i.e. when the material transforms from austenite to martensite it changes from 100% austenite to 100% martensite in one step. The same is also true for the austenite transformation. The thermal dilation is calculated by linear interpolation from a dilation test and hence the response is dependent on the specific conditions of the test, in this case a heating rate of 100°C/s and a cooling rate of 10°C/s, Figure 4.

Figure 4: Dilatation test with a heating rate of 100°C/s and a cooling rate of 10°C/s.
In the second phase evolution model presented, that used in Papers III, IV and V, temperature and time are taken into account when predicting the formation of austenite whilst the transformation of martensite is based on the maximum amount of austenite and temperature. According to Kirkaldy and Venugopalan (1984) the austenite transformation kinetics can be written in general form as:

\[
\frac{dZ_a}{dt} = F_G F_C F_T F_Z
\]  

Where \( F_G \) describes the effect of the austenite grain size; \( F_C \) the effect of the alloy composition; \( F_T \) the effect of the temperature; and \( F_Z \) the effect of the current fraction formed. In the present work the grain size and composition are neglected or rather included in the material constants in the transformation equations discussed later. Later, Oddy et al. (1996) proposed a transformation equation for low carbon steels based on the theory of Kirkaldy and Venugopalan (1984). The model assumes that austenite starts to form when the temperature is above the start of the austenite transformation temperature \( A_{e_1} \), Figure 4, and ends at \( A_{e_3} \). The transformation is described by Eq. (3) to Eq. (5) below and where \( \dot{z}_a \) is the austenite transformation rate, \( z_a \) the volume fraction of austenite, and \( z_{eu} \) the phase equilibrium defined in Eq. (4), \( \tau \) is a function of temperature, \( T \), given by Eq. (5) and \( \tau_0 \), \( \tau_e \), and \( n \) are material constants. The anisothermal formation of austenite is predicted by integration of Eq. (3); the numerical procedure is considered later in this chapter.

\[
\dot{z}_a = n \cdot \left( \ln \left( \frac{z_{eu}}{z_{eu} - z_a} \right) \right)^{\frac{n-1}{n}} \cdot \left( \frac{z_{eu} - z_a}{\tau} \right)
\]

\[
z_{eu} = \frac{T - A_{e_1}}{A_{e_3} - A_{e_1}}
\]

\[
\tau = \tau_0 \cdot \left( T - A_{e_1} \right)^{-\tau_e}
\]

The calculation of martensite transformation is based on Koistinen-Marburger’s equation, Eq. (6), Koistinen and Marburger (1959) and is dependent on the maximum austenite fraction \( z_{a_{\text{max}}} \) and temperature, where it is assumed that the transformation starts at the martensitic start temperature, \( M_s \), Figure 4 and where \( b' \) is a material constant which depends on: composition, crystallography of the martensite habit planes, cooling rate, stress state, and the driving force for the deformation, Ueda et al. (1994). Koistinen-Marburger’s equation has been extended so that \( M_s \) is a linear function of hydrostatic pressure and the equivalent stress, Ueda et al. (1994). This modified model provides a more complex treatment of the phase calculation due to the coupling of stress state and phase evolution. The modified Koistinen-Marburger’s model is not used in this work.

\[
z_m = \left( 1 - e^{-b' (M_s - T)} \right) z_{a_{\text{max}}}
\]
The calculation of thermal dilatation is accomplished by associating a thermal expansion coefficient for each phase with a volumetric transformation strain for each phase transformation. Determination of the coefficient of linear thermal expansion and volumetric transformation strain are examined in the next section as well as the results produced using the evolution equation for austenite and martensite transformation.

Plastic flow arising from changes in the proportions of different phase, in this case during the martensite transformation, in combination with the stress field is known as transformation induced plasticity (TRIP). TRIP is induced in the weaker phase even if the stresses are insufficient to induce classical plasticity; this is often referred to as the Greenwood-Johnson mechanism, Leblond et al. (1989). Also, if a martensitic transformation takes place under an external loading, the martensite plates are formed with a preferred orientation; the Magee mechanism, Leblond et al. (1989). In the current work, any selective orientation in the martensite created due to an external load, i.e. Magee mechanism, is ignored; an assumption also used by Vincent et al. (2005). Leblond et al. (1989) proposed a model for the evolution of TRIP-strain rate, Eq. (7), where empirical data has shown that TRIP-strain evolves in the direction of the deviatoric stress, \( s_{ij} \), Leblond et al. (1989).

\[
\dot{\varepsilon}_{\text{trip}}^{ij} = \frac{3}{2} K' \frac{d\phi}{dz} h \cdot \dot{z} \cdot s_{ij}
\]  

\[
\phi_{\text{Desalos}} = z (2 - z)
\]  

\[
\phi_{\text{Leblond}} = z (1 - \ln z)
\]  

\[
K' = \frac{1}{\sigma_y^a} \frac{\Delta V}{V}
\]  

\[
h = \begin{cases} 
1 & \frac{\sigma}{\sigma_y} < 0.5 \\
1 + 3.5 \cdot \left( \frac{\sigma}{\sigma_y} - 0.5 \right) & \frac{\sigma}{\sigma_y} \geq 0.5
\end{cases}
\]  

Several equations are suggested for \( \phi \) in Eq. (7) where the expression from Desalos (\( \phi = \phi_{\text{Desalos}} \)) Eq. (8) is used in Paper III and the expression from Leblond (\( \phi = \phi_{\text{Leblond}} \)) Eq. (9) is used in Papers IV and V. The expression \( \phi_{\text{Leblond}} \) seems to give the best agreement for the martensitic steel treated here. An expression for \( K' \) is given by Eq. (10) where \( \frac{\Delta V}{V} \) is the relative difference of volume between austenite to martensite resulting from the transformation and \( \sigma_y^a \) is the yield limit of the austenite phase. The function \( h \) in Eq. (7) describes the proportionality between the applied von Mises stress \( \sigma \) and the current yield limit, \( \sigma_y \), according to Leblond et al. (1989), Eq. (11). The yield limit is obtained from Eq. (12) discussed later. In this work is it assumed that TRIP is created only when no plastic flow occur.
4.1.1 Obtaining Parameters and Numerical considerations

The parameters for austenite and martensite transformation used in Eq. (3) to Eq. (6) and presented in Paper III (Table 1) are determined by a curve fitting procedure based on several dilatometric tests. The thermal expansion coefficients are determined from the dilation test by calculating the slope of the linear parts of the dilation curve, \( \alpha_{fp} \) and \( \alpha_a \) in Figure 5 and the transformation strain is determined by the procedure in Figure 5. The thermal expansion and transformation strain are presented in Paper III (Table 2). The transformation rate equation for the austenite transformation Eq.(3) is integrated explicitly and time step splitting is used if the temperature increment becomes large. The calculation of martensite transformation, Eq. (6), is straightforward since it is based on current temperature and maximum austenite fraction \( z_{max}^a \).

A comparison between the dilatometric test and calculated dilatation curves using Eqs.(3) to Eq.(6) and the parameters in Paper III (Table 1 and 2), are shown in Figure 6. The material properties which are assumed to be affected by the phase content and computed by a mixture rule defined in Eq. (12), are thermal dilatation, yield limit, \( \sigma_y \), and hardening parameters, \( H' \). The thermal properties of the material, Young’s modulus, \( E \), and Poisson’s ratio, \( \nu \) are assumed to have the same temperature dependency for all phases. Latent heat due to solid-state transformations is neglected throughout the work, but the latent heat of melting is included. Thermal and mechan-
ical property data are presented Papers I to V, respectively. The material properties affected by phase content are calculated by assigning separate temperature dependent properties to austenite, martensite and the ferrite/pearlite mixture. These properties are then combined using linear mixing rules applied to the macroscopic material properties as used by Börjesson and Lindgren (2001).

\[ Y = z_{fp}Y_{fp} + z_{a}Y_{a} + z_{m}Y_{m} \]  
\[ z_{fp} + z_{a} + z_{m} = 1 \]

Where \( z_{fp} \) is the volume fraction of the ferrite/pearlite mixture, \( z_{a} \) is the volume fraction of austenite and \( z_{m} \) is the volume fraction of martensite. \( Y_{fp} \) is the material property for ferrite/pearlite, \( Y_{a} \) is the material property for austenite and \( Y_{m} \) is the material property for martensite. For calculation of the yield limit using the linear mixture rule, hence:

\[ \sigma_{y} = z_{fp}\sigma_{y}^{fp}\left(H'_{fp}\left(\varepsilon_{ij}^{p}\right)\right) + z_{a}\sigma_{f}^{a}\left(H_{a}^{a}\left(\varepsilon_{ij}^{a}\right)\right) + z_{m}\sigma_{m}^{m}\left(H_{m}^{m}\left(\varepsilon_{ij}^{m}\right)\right) \]

Where \( \sigma_{y}^{fp} \) and \( H'_{fp} \) are the yield limit and hardening modulus for ferrite/pearlite respectively, \( \sigma_{y}^{a} \) and \( H_{a}^{a} \) are the yield limit and hardening modulus for austenite respectively and \( \sigma_{y}^{m} \) and \( H_{m}^{m} \) are the yield limit and hardening modulus for martensite, respectively and \( \varepsilon_{ij}^{p} \) the plastic strain.

Figure 6: Calculated thermal dilatation (x’s) using the Eq. (3) to Eq. (6) and the parameters in Paper III compared to a dilatometric test (solid line).
4.2 Constitutive models

In the mathematical description of material behaviour, the response of the material is characterised by a constitutive equation that gives the stresses as a function of the deformation history of the body. Different constitutive relations make it possible to distinguish between a viscous fluid, rubber, concrete or metal, for example. There is an extensive body of literature on the constitutive equations, for example Lemaitre and Chaboche (1990), Miller (1987) and Stouffer and Dame (1996) which all consider different phenomena and models of elasticity and inelasticity where inelasticity is the generic term for plasticity, viscoplasticity, and creep. The models range from a deviatoric plasticity model using von Mises yield condition and associated flow rule to complex sets of equations like MATMOD, Miller (1987), or Bodner’s model, Bodner and Partom (1975). Bodner’s model and MATMOD and are known as unified models since plasticity/viscoplasticity and creep are combined into the same model. Despite the existence of many constitutive models, a common problem is that material parameters are often lacking. In a subsequent section, a method for a combined approach using a numerical implementation of a constitutive model in a finite element code for material parameter identification is described.

The implementation of the constitutive relation in a finite element code requires a procedure for the evaluation of the stress, the deformation and an algorithm for the integration of the rate form of the constitutive relation. This is called a stress update algorithm. The computational aspects of plasticity are treated in, for example, Simo and Hughes (1997), Belytschko et al. (2000) and Crisfield (1996, 1997) and are discussed later in this chapter. Four basic concepts in elasto-plastic models are the decomposition of the strain into an elastic, reversible part $\varepsilon_{e \sigma}$ and a irreversible plastic part $\varepsilon_{p \sigma}$, a yield function, a plastic flow rule, and an evolution equation for the internal variables such as a hardening rule which governs the evolution of the yield function. Elasto-plastic materials are further classified as rate-independent materials, where the stress is independent of the strain rate, and rate-dependent (viscoplastic) materials in which the stress depends on the strain rate. Figure 7 shows a test where three strain rates are used; the material is clearly rate-dependent. The elastic-plastic models for rate-independent plasticity and viscoplasticity all assume a linear relation between stress and elastic strain; Hooke’s law. The yield criterion or yield surface defines the limit of elastic behaviour i.e. defining when plastic flowing occurs. It is important to note that constitutive equations exist that do not have an elastic domain, for example the Bodner’s model. The flow rule relates the plastic strain increment tensor to the stress state and loading increment. In other words, how the plastic flow occurs. The hardening rule is used to model changes in the yield criterion and flow equation because of inelastic straining i.e. the evolution of the yield surface. Each of these concepts are treated in the following sections.
The decomposition of the elastic and plastic parts can either be through the additive decomposition of the strain rates, Belytschko et al. (2000) or using a multiplicative split of the strain rate, Simo and Hughes (1997). Here, an additive decomposition is used, Eq. (15), where the total strain rate, \( \dot{\varepsilon}_{ij} \), is decomposed into an elastic strain rate, \( \dot{\varepsilon}^e_{ij} \), an inelastic strain rate, \( \dot{\varepsilon}^p_{ij} \), a thermal strain rate, \( \dot{\varepsilon}^{th}_{ij} \), a transformation strain rate, \( \dot{\varepsilon}^{tra}_{ij} \), and a TRIP strain rate \( \dot{\varepsilon}^{trip}_{ij} \), Eq. (15). The material models used in the current work assume that there is no difference between the inelasticity resulting from rate-independent plasticity, viscoplasticity, or creep. Thus, all these contributions can be collected in the plastic strain term:

\[
\dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^p_{ij} + \dot{\varepsilon}^{th}_{ij} + \dot{\varepsilon}^{tra}_{ij} + \dot{\varepsilon}^{trip}_{ij}
\]  

(15)

In a hypoelastic material model, the rate of stress is related to the rate-of-deformation. Hypoelasticity used primarily for representing the elastic response in phenomenological elastic-plastic models where the elastic deformations and dissipative effects are small, Belytschko et al. (2000). The assumption of additive decomposition of the strain rates and the hypoelastic models gives:

\[
\dot{\sigma}_{ij} = C_{ijkl} \dot{\varepsilon}^e_{kl} = C_{ijkl} \left( \dot{\varepsilon}_{kl} - \dot{\varepsilon}^p_{kl} - \dot{\varepsilon}^{th}_{kl} - \dot{\varepsilon}^{tra}_{kl} - \dot{\varepsilon}^{trip}_{kl} \right)
\]  

(16)

Where \( C_{ijkl} \) is the elasticity tensor and \( \dot{\sigma} \) is an objective stress rate as discussed in Bonet and Wood (1997) or Belytschko et al. (2000).
For many metals, the plasticity models depend on shear stress and are independent of mean stress or hydrostatic stress, i.e. deviatoric models or $J_2$-models where $J_2$ is the second stress deviatoric invariant. The yield function, $f$, used in Papers I through V is based on von Mises $J_2$-stress and is defined in Eq. (17) for the rate-independent case and in Eq. (18) for the rate-dependent case. A stress state inside the yield surface, $f < 0$, implies elastic behaviour. However, a stress state on the yield surface, $f = 0$, may imply elastic, neutral, or inelastic loading. To decide which branch is taken during loading/unloading the Kuhn-Tucker condition found in, for example, Simo and Hughes (1997) is used.

$$f_{RI} = \bar{\sigma} - \sigma_y$$  \hspace{1cm} (17)

$$f_{RD} = \bar{\sigma} - \sigma_y - K (\dot{\epsilon}^p)^N$$  \hspace{1cm} (18)

$$\bar{\sigma} = \sqrt{\frac{3}{2}} (s_{ij} - \alpha_{ij}) (s_{ij} - \alpha_{ij}) = \sqrt{3J_2 (s_{ij} - \alpha_{ij})}$$  \hspace{1cm} (19)

$$s_{ij} = \sigma_{ij} - \frac{1}{3} \delta_{ij} \sigma$$  \hspace{1cm} (20)

The yield limit, $\sigma_y$, is usually temperature dependent and its evolution is dependent on the hardening. $\bar{\sigma}$ is the equivalent von Mises stress defined in Eq. (19) where $s_{ij}$ is the deviatoric stress tensor, defined in Eq. (20), $\alpha_{ij}$ is the back stress tensor due to kinematic hardening, and $\dot{\epsilon}^p$ is the equivalent plastic strain rate. $K$ and $N$ in Eq. (18) are temperature dependent material parameters given in Paper III.

Two common types of hardening behaviour are isotropic and kinematic hardening. The isotropic hardening model changes the size of the yield surface whilst the kinematic hardening model translates the yield surface, i.e. changes the backstress. Kinematic hardening is mainly used when the material experience cyclic behaviour. Both types of hardening may include terms for recovery effects but in this work, these terms are omitted. There are many different equations for the evolution of hardening examples can be found in Stouffer and Dame (1996) and Miller (1987). It is assumed that plastic flow is orthogonal to the yield surface and an associated flow rule is thus used throughout the work. The associated flow rule is due to the thermodynamic requirement of maximizing the dissipated energy. Creep models are used in the heat treatment simulation reported in Papers I, III, and IV and is discussed briefly here. The modelling of creep in the current work is considered to be a special case of viscoplasticity without an elastic domain. The first model is a subset of the flow rule given in Eq. (18), where the elastic domain is removed, i.e. $\sigma_y = 0$. This creep model is known as Norton’s law, Eq. (21), and models dislocation creep Stouffer and Dame (1996). The material parameters, $k_{norton}$ and $n_{norton}$, can be obtained directly from a stress relaxation test at the desired temperature.
The creep model used in Paper III, called the Interpolation creep model, is not explicit expressed by an equation but rather is based on uniaxial creep tests carried out at different stress levels and temperatures. During the tests, the strain versus time is measured and the creep strain rate versus accumulated creep strain extracted. The points that define the curves shown in Figure 8 are stored. Given the temperature, stress, and creep strain, known properties in a FE-analysis, the creep strain rate can be found by linear interpolation. This method makes the model stress, temperature, and strain hardening dependent. If different material microstructures (phases) are present, it is no problem to include this parameter in the creep model by simply carrying out supplementary creep tests. A negative aspect with this creep model is the time consuming tests that have to be carried out to acquire enough data, compared to the work required to obtain data for Norton's model.

4.2.1 Obtaining Parameters

Many constitutive models share the common problem of lack of material parameters. In Paper II, a toolbox for evaluation of the constitutive model used together with an optimisation procedure for parameter fitting is presented. In addition, different parameter fitting procedures and optimisation techniques are examined. The toolbox for parameter identification and workbench for loading were implemented in MATLAB. The toolbox is used for preliminary evaluation of a constitutive model and/or
its numerical implementation. The implementation of the constitutive model is used directly when doing parameter identification. The MATLAB tools for optimisation are readily available and it is a simple matter to port the algorithm to the finite element code when the material modelling stage is completed.

Sometimes the parameter identification is straightforward as different parameters can be obtained directly from tests. However, this is not possible for material models whose parameters cannot be easily extracted from test results. In this case, a systematic and objective computer based procedure for parameter identification is necessary. In this section and in Paper II, two parameter fitting procedures are discussed. The first of these, direct parameter fitting, is shown schematically in Figure 9. Direct parameter fitting can be applied for tests such as the uniaxial test, where it is possible to measure over a homogenously deformed volume in order to obtain strain and stress; direct fitting is used in Paper II. The idea in direct parameters fitting is to find the material parameters, $p_{\text{final}}$, that minimise the difference between the measured $\sigma_e$ and computed stress, $\sigma_c$. Different constraints may have to be given for the parameters to find realistic parameters.

The second fitting procedure, inverse modelling, is shown schematically in Figure 9. This method is a more general approach than the direct parameter fitting technique. The idea behind inverse modelling is to use a finite element model of the actual test. In Figure 9, $O$ represents measured quantities obtained from a test, for example stress, strain, and/or friction. The measured quantities are separated into loading (independent quantities), $O_l$, and experimental results (dependent quantities), $O_{re}$. The loading

Figure 9: Parameter fitting with (left) homogenous tests giving stress and strain data directly and (right) with tests where inverse modelling is needed.
Figure 10: Parameter fitting for strain rate jump tests of a material with an initial ferrite/pearlite microstructure. Measured (circles) and computed (line) data.

are also used as input to the finite element model, the results of which are the computed results \( O_{rc} \). The computed results are compared with the measured in order to find the best material parameters.

For the two parameter-fitting procedures discussed, Figure 9, an initial guess must be provided. Comparing results calculated from the guess and measured quantities give an error. If this is greater than some criteria, a new guess should be made. Two optimisation methods, deterministic and stochastic optimisation, can be used to find a new, hopefully better, guesses. The deterministic method is typical some kind of gradient method which can be quite efficient but may find local minima, and is thus dependent on the starting value chosen. Stochastic methods can be some kind of a genetic method which have an underlying logic of survival of the fittest coupled with random generation when creating new guesses for key parameters. Genetic methods are relatively independent of the starting values used but require more iteration. It is common to combine genetic method with gradient methods to obtaining good starting values. In Paper II, different material models, numerical algorithms, and methods for parameter identifications are discussed. Parameter fitting using the viscoplastic model with nonlinear isotropic hardening (later used in Paper III) was carried out on a martensitic stainless steel. A snapshot from the material parameter determination is presented in Figure 10 and all parameters obtained are presented in Paper II.
4.2.2 Numerical considerations

The implementation of the constitutive relationship in a finite element code requires a procedure for the evaluation of the stress due to deformation. The algorithm for the integration of the rate form of the constitutive relation is called a stress update algorithm. The computational aspects of plasticity are treated fully in, for example, Simo and Hughes (1997), Belytschko et al. (2000) or Crisfield (1996, 1997) and are discussed only briefly in this section. Note that useful numerical models have two requirements. The first is accurate, physically realistic relations to describe the physical processes involved and the second is effective numerical procedures.

For the integration of constitutive models in this work, a class of methods called return mapping algorithms, which are consider being robust and accurate, are used. One of the members of this is the radial return method Krieg and Krieg (1977) and is used in Papers I to V. The return mapping schemes consist of an initial elastic-predictor step, involving an excursion (in stress space) away from the yield surface, and a plastic-corrector step, which returns the stress to the updated yield surface. Two components of the method are an integration scheme that transforms the set of equations into a set of nonlinear algebraic equations and a solution scheme for the nonlinear algebraic equations. The solution to the set of nonlinear algebraic equation is typically obtained using a Newton-Raphson procedure and can be based on different integration schemes such as generalised trapezoidal rule, generalised mid-point rule, or Runge-Kutta. In Papers I to V, a fully implicit method based on a backward Euler scheme is used in which the increments in plastic strain and internal variables (if such exist) are calculated at the end of the step and the yield condition is enforced at the end of the step.

Shell elements are used in Papers IV and V in which the assumption of plane stress is used. Plane stress complicates the stress update algorithm somewhat since this enforces an extra condition which must be fulfilled, $\sigma_{33} = 0$. Crisfield (1996) presents a numerical scheme for plasticity in plane stress where the extra condition $\sigma_{33} = 0$ is fulfilled by solving one algebraic equation. This method is used in Paper IV and V.

5 Simulation of manufacturing processes

This chapter discuss the finite element method and the solution methods used in this work. In addition, the modelling of welding and heat treatment with the emphasis on material behaviour and boundary condition are also considered.
The Finite Element Method has been used since the beginning of the 1970's for the simulation of thermo-mechanical manufacturing processes such as welding, Ueda and Yamakawa (1971) and Hibbitt and Marcal (1973). Initially, these simulations were primarily used in the nuclear power industry. Simulations of welding have been further investigated by many researchers, e.g. Goldak and Bibby (1994) and Yang et al. (2002) and several review articles on welding written e.g. Lindgren (2001a,b,c). Industrial products often have a complex shape, which can result in long computational time due to the large simulation models involved. Modelling techniques have been developed to decrease computational time. For example, Rick et al. (1998) and Andersen (2000) carried out welding simulations on large fabricated structures. Andersen used a local/global approach where other numerical techniques such as adaptive meshing, Runnemalm (1999), or parallel computing, Berglund et al. (2001), were used to minimise computational time. In the current work, simulations of welding were carried out in Papers I, III, IV, and V.

Early simulations of heat treatment were carried out by Burnett and Pedovan (1979) and Sjöström (1982). Burnett and Pedovan (1979) calculated residual stresses in case hardened cylinders whilst Sjöström (1982) calculated quench stresses in steel. Rammerstorfer et al. (1981) carried out simulation of the heat treatment process which included creep and phase changes. During the last two decades, many researchers have developed heat treatment simulations to solve quenching problems in steels, e.g. Thuvander (1996) and Silva et al. (2004). The primary intention with these simulations was to predict distortion and residual stresses. Donzella et al. (1995) predicted the residual stresses and microstructure in a solid rail wheel. Simulation models have also been developed to calculate hardness after quenching, Tajima (1996). Simulations combining quenching and tempering were carried out by Ju et al. (1996). In the current work, simulation of heat treatment was carried in Papers I, III, IV, and V. Simulations combining welding and heat treatment are less common. Combined simulations were carried out by Josefson (1982) who calculated the residual stresses after post weld heat treatment of a thin wall pipe. Wang et al. (1998) simulated local post welding heat treatment of a pipe with different heated bands and used a power creep law when simulating stress relaxation.

Doing welding and heat treatment simulation, which encompasses both mechanical and thermal fields, requires some kind of coupling between these fields. There are at least three different ways in which this type of coupling can be carried out. The first is a fully decoupled approach, where the thermal solution is carried out prior to the mechanical solution. This is an acceptable approach if the mechanical boundary conditions do not affect the thermal response of the structure and if plastic dissipated energy can be ignored. The second approach is the so-called staggered approach where
the geometry of the thermal solution lags one step behind the mechanical solution. In welding simulation, small time steps are usually used and the staggered approach believed to be sufficient. The staggered approach is used for all welding and heat treatment simulation in this work. The third approach, which is the most rigorous, is a fully coupled analysis between the thermal and mechanical fields, where solutions are computed for the thermal and mechanical variables simultaneously.

Using the finite element method for transient problems, one of two methods schemes can be used, explicit or implicit time stepping schemes. The majority of welding and heat treatment simulations reported in the literature have been solved using implicit time stepping. The explicit method is commonly used in problem with short duration or time scales, for example in crash analyses or for forming problem analyses excluding springback. The implicit method is used in all welding and heat treatment analyses in the current work, except the fluid dynamics analysis carried out in Paper I. Using the implicit method the solution is obtained by an iterative procedure. This is discussed, for instance, in Crisfield (1996). The iterative procedure used is usually a variant of the Newton-Raphson procedure. The linear system of equations obtained can be solved either by a direct sparse or iterative solver.

In summary, an implicit time stepping method and the updated Lagrange procedure has been used for the thermo-mechanical simulations presented in the current work. For the fluid mechanics analysis carried out in Paper I, an explicit time stepping method with a Eulerian frame was used.

5.1 Simulation of welding

This section discusses thermal and material modelling and welding simulation with an emphasis on heat source modelling, treatment of welding filler material and material behaviour. In the welding method studied in this work, an electric arc is used to melt the material. The general process consists of an electrical field between the anode and the cathode surrounded by an ionised gas. The complex phenomena surrounding the arc are not fully understood and include, for example, plasma flow, fluid flow and surface tension in the melted material, electro-magnetic fields, phase transition (liquid-solid states), and solidification. The temperature in the weld pool is approximately 3000-4000°C. Due to the extremely complex phenomena associated with arc welding, simplifications have to be made. Fortunately, the complexity of the weld pool dynamics is no obstacle as far as modelling the macroscopic effects of welding is concerned. Only the shape of the weld pool and the amount of energy transferred were used in the models of the welding process developed in this work. The heat source description used in the present work is the double ellipsoidal power density distribution suggested by Goldak
and Bibby (1994). Heat input in the welding simulation is modelled as a travelling heat source and calibrated, i.e. the process of determining of the parameters describing the heat distribution uses the dimension of the fusion zone (FZ). This method of calibrating temperatures was in very good agreement with the measured temperatures presented in Lundbäck et al. (2003). The calibration of the heat source is discussed further in Paper V.

5.1.1 Material Behaviour

The technique of activating elements was used to imitate the joining of material in the three-dimensional models presented in Papers IV and V. With this technique, one row of elements along the weld path is initially deactivated. The deactivated elements do not contribute to the stiffness matrix but are active in the thermal part of the simulation. The volume of the inactivated elements corresponds to the amount of filler material added during the welding sequence. The elements are activated in the mechanical part of the simulation when the temperature rises above the melting point of the material and the temperature is decreasing ($\frac{dT}{dt} < 0$). The elements then adopt the mechanical properties of the material corresponding to the current temperature.

![Figure 11: Gap deformation history during butt-welding of two plates using different minimum yield limits in the simulation compared with a test, from Paper V.](image)

Figure 11: Gap deformation history during butt-welding of two plates using different minimum yield limits in the simulation compared with a test, from Paper V.
A somewhat different approach is used to model the filler material for the axisymmetric models presented in Papers I, III, and IV. The behaviour of the filler material is simulated by giving the volume corresponding to the filler material a low yield limit and zero thermal dilatation until the temperature has passed melting point and the temperature is decreasing \((\frac{dT}{dt} < 0)\). This method minimises effects on the structure before the temperature has reached the melting point, at which point the elements are given normal properties. In all models, the plastic strains are set to zero when the material reaches its melting point and for as long as the temperature is above the melting point.

In all simulations carried out in the present work, it is assumed that the material from the filler wire have the melting temperature when it first meets the material surface. Common for the three-dimensional and axisymmetric treatments of filler material are that the melted material is treated as a soft solid, i.e. the stiffness, Young’s modulus and yield limit are assigned low values. However, material properties can only be decreased to a certain level. If they are too low, then problems occur in the numerical simulations. It was discovered in the current work that the values used affect the results in the case of flexible structures i.e. structures that have very little restraint during welding and where large deformations occur. The importance of high temperature modelling of the yield limit on the gap deformation behaviour during the butt-welding of a plate is shown in Figure 11.

The Satoh test imitates the heating and cooling cycle that occurs during welding Satoh (1972). This kind of test can also be used to investigate the behaviour of different material models or for validation of models and is part of the validation scheme presented in the next chapter. The Satoh test was designed to recreate the temperature and stress cycle experienced by the material during welding. In a Satoh test, the specimen is clamped at the ends in a test rig, then heated, and subsequently cooled, Figure 12. The reaction force is recorded during this thermal cycle. The Satoh test carried out here, was modified in the experiments carried out in this work by prescribing the displacement of one of the clamps instead of using completely fixed clamps. This was done in order to obtain a stable force response in the test equipment. The temperature history associated with the test and the stress response, where the stresses are averaged by knowing the force and area of the thinner section are shown in Figure 12. The Satoh test was simulated using different material models, which are shown in Figure 12.

It was found in Paper V that the initial geometry is an important variable in the analysis of welded flexible structures like the set-up shown in Figure 13. The influence of the initial geometry on the out-of-plane (z-direction in Figure 13) deformation is
investigated in Paper V using welding simulations where the simulation model is given an initial butterfly angle of 0° and 1°. The definition of the butterfly-angle is given in Paper V (Figure 19). When it became clear that butterfly angle was important, a new experiment was carried out. The experimental set-up was similar to that used in Paper V. The only difference between the experiments is that the plates were given an initial butterfly-angle of +4°.

The transient out-of-plane deformation of the plate in the experiments was measured and compared with deformation from welding simulations in Figure 13. The zero point for measurement of deformations is at (140.9,45.1) using the coordinate system shown in Figure 11 in Paper V. All the plates welded in the experiments showed similar deformation behaviour, i.e. all had out-of-plane deformation in the same direction. This was not the behaviour of the plates in the experiments carried out in Paper V; see Figure 15 in Paper V. However, misalignment between the plates is still a problem as can be seen in Figure 15 in Paper V. The measured out-of-plane deformation presented in Figure 13 is the average deformation of five welding tests using a fixture with an initial butterfly of +4°. The results from welding simulations are also shown in Figure 13. These simulations were carried out using several material models; the acronyms for the material models are found in Paper III (Table3). In addition, it was found that the RIM-model gave the maximum negative deformation and RDM-model the minimum negative residual out-of-plane deformation, Figure 13.
Figure 13: Welding of a plate (190x100x1.7 mm when welded). Left: 1 indicates start of weld and 2 indicates end of the weld. Right: Deformation out-of-plane (z-direction) using different material models compared with test results. The acronyms used for the material models are found in Paper III (Table 3).

An investigation into the influence of the choice of material model used was also carried out in Paper III on an aerospace component. These simulations of the welding process showed that minimum negative deformations are obtained using viscoplastic models, i.e. the RDM or the RDMT-model. In addition, maximum negative residual deformations were obtained using a rate-independent model, i.e. RIM or the RIMT-model. It can be seen in Paper III that the inclusion of TRIP has a small effect on the deformation behaviour. An examination of how different levels of discretisation affect deformation behaviour in the welding and heat treatment simulations is presented in Paper IV. The two discretisations used in Paper IV are the axisymmetric model from Papers I and III and a three-dimensional shell model. The predicted residual deformation due to welding was improved using the three-dimensional model, Figure 14, based on measurements of residual deformations after each weld not presented in this work owing to confidentiality issues.

In Paper V, measurements of the residual stresses due to welding were carried out using a hole-drilling technique. This paper also presents simulations of welding using the RIMT-model and compares measured and simulated residual stresses. An additional welding simulation using the RIM-model is included here for comparison with measurements, Figure 15. The principle difference between the results obtain with
the different models is that the peak stresses are larger for the RIM-model compared to the RIMT-model in the heat-affected-zone (HAZ) and the fusion zone (FZ). An examination of how different levels of discretisation affects residual stresses due to welding and heat treatment is presented in Paper IV.

5.2 Simulation of post weld heat treatment

This section considers modelling of the heat treatment process. The first section covers material modelling for heat treatment and the second modelling of boundary conditions during the heating and cooling sequence. The heat treatment cycle has been divided into three parts, Figure 1 – radiant heating, a holding phase where most of the stress relieving takes place and cooling by circulating a cold gas.

5.2.1 Material Behaviour

The material model must account for the physical process involved in the heat treatment with sufficient accuracy to provide the required results. In the present work, two procedures for including creep in the heat treatment simulation are used, Figure 16. In the first model, denoted Creep1-model in Figure 16 and used in Papers I and III, a rate-independent plastic model, was used for the heating and cooling sequence and a
creep model used for the holding sequence to simulate the relaxation of stresses. In the second model (Creep2-model in Figure 16 and presented and used in Papers III and V) a creep model together with the rate-independent model was used for all sequences in the heat treatment simulation. The difference in response using the different procedures is minor and is shown in Corrigendum to Paper III (Figure 3).

Stress relaxation tests can be used to validate creep models under conditions similar to stress relief heat treatment and are used in the validation scheme presented in the next chapter. A compression test was carried out on a cylindrical test specimen fixed at one end and with a varying force applied at the other end. The load varies with temperature, as shown in Figure 17. Force and change in diameter are recorded during the test. The radial strain is calculated from the change in diameter divided by the original diameter. An axisymmetric model together with the interpolation creep model presented in Chapter 4 was used in the simulation and the predicted results compared with the test result shown in Figure 17.

In Paper V, measurements of the residual stresses due to welding were carried out using a hole-drilling technique. Although no measurements of the residual stresses

Figure 15: Predicted residual stresses using the RIM and RIMT-model and measured residual stresses (circles with error bars) after welding. The left-hand side of the diagram shows the stresses in the longitudinal (x), welding, direction and the right-hand side, the stresses in the transverse (y) direction; the directions are those given in Figure 13.
after heat treatment were included in Paper V. Such measurements have been carried out and are presented here. The heat treatment simulation of a plate was carried out according to the method presented in Paper V. The RIMT-model was used for the welding simulation and preceded the heat treatment simulation. Comparing the predicted residual stresses with the measured showed that the longitudinal stresses and the transverse stresses were predicted with good accuracy by the simulation, Figure 18.

It has also been observed, by measurements, that the residual stresses after heat treatment are affected by the initial geometry.

Figure 16: Different procedures for applying the interpolation creep model.

Figure 17: Temperature and stress history for creep test and results from a creep test and analysis using the interpolation creep model of the same test, from Paper V.
Figure 18: Predicted residual stresses using the interpolation creep model and measured residual stresses (circles with error bars) after heat treatment. The left-hand side of the diagram shows the stresses in the longitudinal (x), welding, direction and the right-hand side, the stresses in the transverse (y) direction; directions as in Figure 13.

An examination of how different discretisations affect residual stresses is presented in Paper IV, as discussed in a preceding section. The examination carried out in Paper IV shows that the residual deformations after heat treatment were more accurately predicted when using the three-dimensional model, Paper IV (Figure 5 and Table 2) when comparing measurements of residual deformations after the heat treatment not presented in this work owing to confidentiality issues.

5.2.2 Boundary Conditions

An important topic in heat treatment simulations is how well the boundary conditions in the model correlate with the actual process. The mechanical boundary conditions are often quite straightforward since the component is often simply positioned on a grid or a plate during the heat treatment. However, the thermal boundary conditions are more complex.

The temperature increase during the heating sequence is the result of heating by radiating elements in the furnace and transferred to the component by thermal radiation and/or convection, as described in Chapter 2. Heating by thermal radiation is modelled and used in Papers I, III, IV and V. Temperature is closely controlled
during heat treatment and can include different heating rates over different temperature intervals and may also include plateau where the temperature is held constant in order to obtain a more even distribution of temperatures in a geometrically complex component, Figure 1.

The FE-software used for the heat treatment simulations in the current work, MSC.Marc – MSC.Software (2003), has functionality for calculating the radiative heat transfer. The radiative heat transfer is modelled by Eq. (22), where $q_{rad}$ is the radiative heat flux, $\varepsilon_{rad}$ is the emissivity, $\sigma_{SB}$ is Stefan-Boltzmann’s constant, $F$ is the viewfactor defined in Eq. (23) and Figure 19, and $T_1$ and $T_2$ are the temperatures of the bodies’ surfaces experiencing the heat transfer, respectively, Figure 19. The viewfactor is the ratio between how much different bodies “see” each other.

$$q_{rad} = \varepsilon_{rad}\sigma_{SB}F(T_1^4 - T_2^4)$$

$$F = \frac{1}{A_1} \int_{A_1} \int_{A_2} \frac{\cos \phi_1 \cos \phi_2}{\pi r^2} dA_2 dA_1$$

(During the cooling sequence, the heat transfer includes convective heat transfer. If radiative heat transfer is thought to be important, it can be included as described earlier in this section. The amount of energy transferred by convection, $q_{conv}$, is primarily dependent on two parameters, Eq. (24). The first parameter is the temperature difference between the component surface and its surrounding, $\Delta T$, and the second is the heat transfer coefficient, $h$. The heat transfer coefficient is dependent on conditions in the boundary layer, which is influenced by surface geometry, the nature of the fluid motion and an assortment of fluid thermodynamic and transport properties, Incropera and DeWitt (1996).

$$q_{conv} = h\Delta T$$
In Paper I, a method was developed and analyses carried out to obtain an approximate distribution for the heat transfer coefficient when an aerospace component is cooled in a heat treatment furnace. The simulation was carried out in two stages; first, the fluid flow was solved using a Computational Fluid Dynamics (CFD) code, FLUENT, using a model like the one shown in Figure 20. The fluid flow analysis was carried out on a three-dimensional model with the boundary conditions given in Paper I. Figure 20 shows the velocity profile and heat transfer coefficient from a simulation in FLUENT. The solution for the heat transfer coefficient is processed to give the boundary condition using Eq. (24) in the thermo-mechanical finite element analysis. Hence, the coupling is accomplished in two steps:

1. Simulation of the fluid flow problem and computation of the convective heat transfer coefficient $h$ in Eq. (24).

2. Applying the heat transfer coefficient, $h$, from step I to the FE-model, as a boundary condition using Eq. (24) in the simulation of the thermo-mechanical problem.

Figure 20: Left: The gas flow in a heat treatment furnace during the cooling sequence. Right: The heat transfer coefficient calculated from the flow in Figure 20 (left).

The inclusion of the computed convective heat transfer coefficient into the finite element model was achieved using user-defined subroutines. The coupling was one-way and it was assumed that any deformations did not affect gas flow in the furnace during cooling. The largest deformations predicted by the simulations were about 3 mm. Similar simulations have been carried out by, for example, Lind et al. (1998) who used fluid mechanics simulations to obtain an approximate distribution of the heat transfer coefficient when quenching a steel cylinder in a gas cooled furnace.
6 Validation of simulation models

Verification and validation (V&V) are the primary methods used to assess the accuracy and reliability of computational simulations. Due to the impact that modelling and simulation predictions can have, the creditability of the computational results is of great concern to engineering designers, managers and those affected by any decisions based on the predictions. In this chapter, a validation strategy for a welding and post weld heat treatment models is presented. The basis for the strategy presented in this work is the paper by Oberkampf (2002) in which the authors present a historical review of V&V, introduce and give different definitions of V&V, and give strategies and guidelines for V&V. Oberkampf (2002) developed the methodology for V&V for computational fluid dynamics (CFD) but stated that the methodology could easily be extended to other disciplines. The methodology is based on the idea that a complete system is too complex and too expensive to use for validation tests or as Oberkampf (2002) expresses it,

"Because of the infeasibility and impracticability of conducting true validation experiments on most complex system, the recommended method is to use a building-block approach."

The recommended validation strategy employs a hierarchical methodology that segregates and simplifies the physical and coupling phenomena involved in complex engineering systems; the decomposition being used to isolate particular phenomena. This hierarchy consists of four levels; system level, subsystem level, benchmark level and unit problem level, Figure 21.

Defining the subsystems involves decomposition of the complete system into more manageable parts where a limited number of the physical processes are involved. In a mechanical analysis, for example, this could involve identifying parts of the system which experiencing conditions typical for the complete model. When carrying out the decomposition, it is of great importance that the cases chosen characterise the phenomena associated with the process being simulated and that the subsystem effectively reveals any weaknesses in the model. Unit cases are used for evaluation of mathematical models covering one physical phenomenon. Benchmark cases involve isolation of a limited number of physical processes, and where special hardware or test fixtures are fabricated to represent the main features of each subsystem. The number of physical processes involved should be less than the number of processes in the subsystem case.

One way to validate models is to compare the result from a computational model with the behaviour of the real structure. Such a comparison gives information about the quality of the simulation, but does not give any useful information as to the source of errors if the simulation and reality do not agree. Oberkampf (2002) criticise the
graphical validation used in many papers, i.e. comparison of computational results and experimental data on a graph. As an alternative, they present several validation metrics, $V$, which give a measure of the error in a single number independent of the data based on a tangent hyperbolic expression. Perfect agreement between the properties compared will give a validation metric of one whilst a value of zero represents an error approaching infinity. One of the equations used to calculate this metric is presented here, Eq. (25), where $Y(x_i)$ are experimental measurements at spatial coordinate $x_i$ and $y(x_i)$ is the predicted value. Validation metrics can be used for hypothesis testing or qualification, Oberkampf (2002). Due to the criticism of the simple graphical validation method, comparisons between measured data and prediction from the simulations preformed in Paper V or Chapter 5 are re-examined in the next section using the validation metric, in Eq. (26), where $x$ is a chosen fixed point on the structure and $t_i$ is the time during which the measured value varies.

$$V = 1 - \frac{1}{N} \sum_{i=1}^{N} \tanh \left| \frac{y(x_i) - Y(x_i)}{Y(x_i)} \right|$$

$$V = 1 - \frac{1}{N} \sum_{i=1}^{N} \tanh \left| \frac{y(x, t_i) - Y(x, t_i)}{Y(x, t_i)} \right|$$

6.1 The proposed validation model

This section describes the proposed validation process for welding and post weld heat treatment, i.e. the validation cases used and the measured quantities used for validation, Figure 22. The validation of the welding and post weld heat treatment processes
is divided into two cases; a benchmark case and a subsystem case. No unit case is used, but calibration tests are included in the description. The quantities evaluated include deformations and residual stresses after welding and deformations and stresses after post weld heat treatment. It would be an advantage to be able to measure transient parameters, but this was not possible during the heat treatment.

The benchmark case chosen for welding is the modified Satoh test and for heat treatment the relaxation test the temperatures and stresses presented in Chapter 5, Figure 12 and Figure 17 respectively. In the benchmark case, a material model is validated using a specially manufactured specimen and known boundary conditions. The results from the benchmark case were only validated quantitatively in Paper V. This validation is re-examined here using the validation metric given in Eq. (26). Comparing the predicted stresses using different material models with measured stresses from the Satoh test shows that the RI-model is rated highest and RDM-model is rated lowest, Table 1. The stress relaxation test was only compared with one model. This metric is also shown in Table 1.

The plate presented in Chapter 5 and Paper V was chosen as a suitable subsystem for validation of welding and heat treatment, Figure 13 in Chapter 5 and Figure 11 in Paper V. The thermal boundary conditions and process parameters were validated using the subsystem case. Transient deformations or residual deformations and residual stresses were used as validation parameters for welding and the transient surface temperature, residual deformations, and residual stresses used as validation parameters for heat treatment.
Table 1: Validation metric for transient stresses in the benchmark cases.

<table>
<thead>
<tr>
<th>Benchmark case</th>
<th>Material model</th>
<th>Validation metric, $V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RI</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>RIM</td>
<td>0.30</td>
<td></td>
</tr>
<tr>
<td>Satoh test</td>
<td>RIMT</td>
<td>0.30</td>
</tr>
<tr>
<td></td>
<td>RDM</td>
<td>0.27</td>
</tr>
<tr>
<td></td>
<td>RDMT</td>
<td>0.27</td>
</tr>
<tr>
<td>Stress reaxation test</td>
<td>Interpolation creep model</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Table 2: Validation metric for out-of-plane deformation of the subsystem case for welding.

<table>
<thead>
<tr>
<th>Material model</th>
<th>Validation metric, $V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RIM</td>
<td>0.51</td>
</tr>
<tr>
<td>RIMT</td>
<td>0.58</td>
</tr>
<tr>
<td>RDM</td>
<td>0.67</td>
</tr>
<tr>
<td>RDMT</td>
<td>0.66</td>
</tr>
</tbody>
</table>

Qualitative validation by graphical comparison was used in Paper V. The measured and predicted transient deformations for the modified set-up, Figure 13, are re-validated here using the validation metric, Eq.(26). Comparing the material models used for analysing the welding of the plate in the modified set-up, Table 2, shows that the RDM-model is rated highest and RIM-model is rated lowest.

7 Summaries of appended papers

Five papers and one corrigendum are appended with this thesis. A summary and the main results from each paper and the relation of each paper to the thesis are given below.

7.1 Paper I

Summary: This paper presents a method for and the results from combined simulation of welding and heat treatment and results from a simulation. The material model required temperature and phase dependent thermal and mechanical properties. Modelling of heat input was accomplished using a double ellipsoid heat input model. However, modelling the heat transfer during heat treatment required a more advanced
strategy and results from a computational fluid dynamics analysis were used to predict the heat transfer coefficients of the component’s surface during the cooling part of the heat treatment sequence.

Relation to thesis: This paper presents a simulation method for combined welding and stress relief heat treatment analysis, which includes the effects of the gas flow in a heat treatment furnace during the cooling sequence.

Results: The simulations revealed that the first two welding operations, where the structure is relatively unrestrained, have the greatest effect on the dimensional parameter of interest. It was found that the cooling part of the heat treatment process does not give rise to any additional plastic strains. In this paper, it was proposed that a three-dimensional model is needed in order to obtain more accurate predictions for the welding process. It was also suggested that using a temperature dependent creep law would improve the simulation of transient behaviour occurring during the heat-treatment process. The input parameters for such a model must be obtained from creep tests carried out over a range of temperatures.

7.2 Paper II

Summary: This paper presents an approach where the numerical implementation of a constitutive model used in the finite element code was also used for material parameter identification. The toolbox for parameter identification was developed using MATLAB, which has the optimisation tools needed for the parameter determination process. Other useful facilities also helped motivate the choice of platform for the implementation of the toolbox. In the paper, different material models, numerical algorithms and methods for parameter identifications are discussed to set the general context and the application of the toolbox for Greek Ascoloy described. The paper presents results from parameter fitting using a viscoplastic model with nonlinear, isotropic hardening. An optimisation strategy of the ”divide and conquer” type was necessary to obtain the seven material parameters required for the chosen model.

Relation to thesis: The parameters obtained for the viscoplastic model with nonlinear isotropic hardening are used in several simulations carried out in thesis.

Results: The toolbox approach is an efficient one for testing and evaluating constitutive models. The efficiency is mainly due to the built-in functions available in MATLAB. Flexibility in imposing constraints other than the common upper and lower limits is very useful. Also, when a reduction of parameter space is carried out, decreased sensitivity to the choice of starting values and increase in optimisation speed were obtained.
7.3 Paper III

Summary: A major concern when carrying out welding and heat treatment simulations is to accurately model material behaviour since this varies with temperature and composition. This paper compares the results obtained using several different material models when simulating welding and heat treatment. The material models include a number of effects such as rate-independence, and viscoplasticity and include phase calculations and TRIP. Two creep models, one of them temperature dependent, and two ways to apply the creep models were investigated.

Relation to thesis: The paper investigates the deformations and residual stresses due to welding and heat treatment when different phenomena are included in the material modelling.

Results: As in Paper I, the simulations revealed that the two first welding operations have the greatest effect on the dimensional parameter of interest and that the cooling stage of the heat treatment process does not give rise to any additional plastic strains.

7.4 Corrigendum to Paper III

Summary: In Paper III, an error in the dilatation model was found where the transformation strain for the austenite to martensite transformation was accidentally put to zero. The estimated value of the transformation strain is 0.006. This was corrected and new simulations of welding and heat treatment carried out.

Relation to thesis: Corrects an error made in the dilatation model in Paper III.

Results: The conclusions given in Paper III do not changed as a consequence of the new results and no new conclusions were included in the Corrigendum. However, a discussion of the differences in the results obtained in Paper III and the Corrigendum is presented.

7.5 Paper IV

Summary: In Papers I and III, a model combining welding and heat treatment simulations of the component is developed and several material models which included phase change effects compared. These simulations were carried out using an axisymmetric finite element model. Results from a three-dimensional shell element model of the same aerospace component as used in Papers I and III was presented in Paper V. The results are compared with the previously used axisymmetric model.

Relation to thesis: The paper examines the differences between an axisymmetric and a three-dimensional model on deformation and residual stresses when doing simulations of combined welding and heat treatment.

Results: From the simulation, it could be concluded that the three-dimensional model gave a better prediction of the dimension of interest compared to results from the ax-
isymmetric model. Actual measurements are not given in the paper owing to confidentiality issues.

7.6 Paper V

Summary: Doing large-scale tests is costly and time consuming and simulation tools are therefore needed to support an effective product development process. Due to the impact that modelling and simulation prediction can have, the creditability of the computational results is of great concern to engineering designers, managers and those affected by decisions based on these predictions. In this paper, a validation scheme is proposed and exemplified for thermal-mechanical models of welding and post weld heat treatment. The validation process presented is divided into two steps; material validation and process validation. Decomposing the validation process in this way has the advantage of qualifying the material model before the manufacturing process is simulated. The focus of the process validation step (subsystem case) is on the loads and boundary conditions in the process. If the welding process is changed, but the material remains the same, it is only necessary to repeat the process validation. However, material and process validation has to be carried out whenever a new material is to be qualified even if the welding process remains the same.

Relation to thesis: The paper presents a validation methodology for thermo-mechanical models of welding and post weld heat treatment. The problem of robustness and sensitivity to high temperature behaviour was noted when simulating welding of structures with little restraint.

Results: Comparing simulations using shell elements with experimental results showed good agreement as far as residual stresses after welding were concerned but an overestimation of the out-of-plane deformations for the simulation of welding and heat treatment. The simulations showed that out-of-plane deformation is strongly influenced by the initial geometry. However, the residual stresses after welding are well predicted by the model.

8 Conclusion and future work

The ability to predict residual stresses and deformations due to fabrication is useful for producers of aero-engine components and may also be beneficial in many other industries. This thesis deals with the simulation of welding and heat treatment, in particular with the modelling of material behaviour and boundary conditions. The work covers numerical and experimental investigations, although the emphasis is on the former. The most important features of the work and the main conclusion are summarized here, together with the author’s opinion on the direction of future work.
The model proposed in this work and the associated methodology provides the means to simulate the welding and post weld heat treatment of aero-engine components. This covers prediction of thermo-mechanical behaviours such as stresses and deformations occurring during welding and subsequent heat treatment in gas-cooled vacuum furnaces.

The methodology indicates how the model can be adapted for new welding and heat treatment processes as well as other materials and also includes calibration and validation procedures.

The welding model is expected to give the adequate accuracy required for predicting deformation and residual stresses at all stages of product and manufacturing development, Figure 3.

The model and methodology have been implemented, tested and are presently in use at Volvo Aero for product and manufacturing development and in also for workshop troubleshooting. For example the welding model has been used to help minimise deformations due to changes in the weld sequence, Voutchkov et al. (2005), for an existing component. The model has also been used in the optimisation of deformations due to welding in a product development project with a new product at Volvo Aero. The welding model is also expected to give adequate accuracy for the results to be used as input to fatigue life analyses.

The heat treatment model is expected to give adequate accuracy when predicting residual deformations and stresses resulting from stress relief heat treatment for it to be used in the two first stages of product and manufacturing development, Figure 3.

Finally, the model for welding and heat treatment can be used to predict whether stability problems such as buckling may occur. It is important to avoid such problems in order to ensure a robust manufacturing process.

Further research is needed for the stress relief heat treatment process to obtain adequate accuracy for all stages of product and manufacturing development. Also, quenching processes can be modelled if calibration of the creep model is made for temperatures higher than those used in the current work. The interaction between phase transformation and creep needs further investigation. Furthermore, a validation procedure for heat treatment independent of welding would be preferable. This should be based on knowledge of the initial state of stresses and deformations. Additionally, data obtained from measurement of transient deformation or strains during the actual heat treatment process would be valuable. The current work focuses on stresses and deformations. However, cracking is another important issue and development of techniques to predict cracking would be of significant industrial interest.
9 Scientific contributions

There are several papers in the literature that describe models of welding or heat treatment. However, few papers have been found that deal with both processes. The use of computational fluid dynamics to obtain realistic boundary condition for the thermo-mechanical simulation of heat treatment on geometrically complex structures has not been found in the literature. The validation methodology presented for welding and heat treatment simulations is unique, to the authors knowledge, and a valuable contribution in helping to facilitate the industrial application of the models. This methodology is a joint contribution together with co-author Daniel Berglund, Berglund (2003). In the introductory part of the thesis the author proposed an approach for quantifying the validation.

References


Paper I

Simulation of Welding and Stress Relief Heat Treatment of an Aero Engine Component
Simulation of welding and stress relief heat treatment of an aero engine component

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Abstract

It is important to control key dimensions in aero engine components during manufacture. This is achieved by finding a stable process-parameter window for each manufacturing operation and to choose an order of manufacture which give an adequate result. Production planning has traditionally been carried out from experience and experiments. However, in order to reduce lead-time and cost, computer based numerical simulations using the finite element method is increasingly being used. Simulations can give valuable information about component dimensions, shape, and residual stresses after each manufacturing process. This paper presents a method and the results of a simulation where welding and stress relief heat treatment operations are combined. Computational fluid dynamics was also used to estimate the heat transfer coefficient of the component’s surface during the heat treatment. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: FEM; CFD; Welding; Stress relief heat treatment; Aero engine

1. Introduction

Welding and heat treatment are commonly used in the aerospace industry. However, these processes can generate unwanted stresses and deformations, a fact that has to be taken into consideration when designing or changing the sequence of manufacturing for a given component. Whilst previous experience can offer some help, costly and time consuming experiments are often required to evaluate component design, material selection, and manufacturing schedules. Pressures to decrease product

development time has created a need for more efficient tools to predict the effect of manufacturing
tools and processes on the final shape and properties of a component.

A long-term aim for Volvo Aero Corporation is to develop simulation tools that can be used
to reliably predict the final properties and shape of a component. One important development is
to integrate the results from simulations of individual manufacturing processes in order to predict
the final shape and residual stresses in a component. Examples where this is important include
making service life predictions based on residual stresses from manufacturing in combination with
the stresses from in-service loads or checking whether design tolerances are met.

Combined manufacturing simulation also allows optimisation of the entire manufacturing process
instead of trying to optimise each individual process, which can give sub-optimal overall results.
For example, the deformation due to stress relief heat treatment is strongly dependent on residual
stresses resulting from a welding process. In this case, optimisation of the welding procedures does
not guarantee an acceptable shape for the component after heat treatment.

The finite element method (FEM) has been used since the early 1970s to predict stresses and
deformations due to welding [1–3]. This tool was primarily used in the nuclear power industry but
is now also commonly used by aerospace manufacturing companies. Roberts et al. [4] used FEM sim-
ulations to develop a process model for electron beam welding that predicted the residual stresses and
distortion with acceptable accuracy. Aero engine components usually have a complex shape, this can
result in long-computational time due to the large-simulation models involved. Modelling techniques
have been developed to decrease computational time. For example, Rick et al. [5] and Andersen [6]
carried out welding simulations on large-fabricated structures. Andersen used a local/global approach
where simulation results from a detailed solid model were mapped onto a global shell model. Other
numerical techniques used to minimise computational time include adaptive meshing Runnemalm
et al. [7] or parallel computing Berglund et al. [8,5].

Detailed heat treatment simulations have been carried out before. For example Donzella et al.
[9] predicted the residual stresses and microstructure in a solid rail wheel whilst Thuvander’s [10]
simulation of distortion due to quenching showed good correlation with measured results. Combined
welding and heat treatment analysis has been carried out by, for example, Josefson [11] who calcul-
ated the residual stresses after post-weld heat treatment of a thin wall pipe. Wang [12] simulated
local post-heat treatment of a pipe with different heated bands and used a power creep law when
simulating the heat treatment process. Chandra et al. [13] developed a methodology for simulating
the complete manufacturing sequence for a complex shaped part. The methodology covered forging,
heat treatment and machining but did not include welding.

A major concern in heat treatment analysis is how well the boundary conditions in the model
 correlate with the actual process. For example, correctly modelling the heat transfer from the sur-
roundings is necessary to predict the correct temperature gradients in the component. The amount
of energy transferred from the surroundings is dependent on two major parameters; the temperature
difference between the component surface and the surrounding and the heat transfer coefficient. Lind
et al. [14] used computational fluid dynamics (CFD) simulations to obtain an approximate distribution
of the surface heat transfer coefficient when quenching a steel cylinder in a gas cooled furnace.

This paper presents a simulation method for combined welding and heat treatment analysis of
martensitic stainless steel components and the use of computational fluid dynamics to obtain an
approximation of the heat transfer coefficient of the component’s surface during the heat treatment
process.
2. Manufacturing and simulation of aerospace components

The Turbine Exhaust Case (TEC) V2500, a fabricated structure made of a martensitic stainless steel, is manufactured at Volvo Aero. One part of the TEC V2500 is the hub, see Fig. 1.

The hub is fabricated by welding two discs, the front- and rear supports, between the bearing housing and the inner ring. The sequence of the different manufacturing steps is shown in Fig. 2. The work presented in this paper has concentrated on the welding and heat treatment processes. A more detailed description of each process is presented in Sections 4 and 5 in this paper.

The component is welded using gas tungsten arc welding (GTAW) with additional filler material. Fabrication begins by welding the rear support, welds A and B in Fig. 3. (See also Fig. 1.) Thereafter, welds D and C on the front support are made. The component parts are first tack-welded together before the final welds are made. The component is heat treated after welding in order to reduce residual stresses. The objective of the simulation presented in this paper was to investigate the deformation behaviour during the different manufacturing steps and hence to predict the final shape of the component.

A key dimension in the final hub is the axial distance $a$ between the bearing housing and the flange on the Inner ring, see Fig. 3a. The simulation reveal which of the manufacturing steps had the largest influence on the key dimension.

![Fig. 1. Part of the TEC V2500, (a) back view and (b) front view.](image)

![Fig. 2. Key manufacturing steps for the hub.](image)
3. Material properties

The material properties and models used are described in the following section. Firstly, the microstructure and thermal dilatation are discussed followed by the mechanical and thermal properties of the material.

3.1. Microstructure and thermal dilatation

The material’s initial microstructure consists of a mixture of ferrite and pearlite. In the numerical model the ferrite/pearlite to austenite transformation is assumed to occur only if the highest temperature experienced by the material was greater than the $A_{e3}$ temperature, see Point 1 in Fig. 4a. Since the cooling rate of any austenite phase formed during welding is always higher than 0.3°C/s between the $A_{e3}$ and martensite start temperature it can safely be assumed that all the austenite is transformed to martensite irrespective of cooling rate. This assumption supported by Fig. 4 which
Fig. 5. Temperature dependent mechanical properties: (a) Young’s modulus, $E$, and Poisson’s ratio, $\nu$ and (b) Temperature dependent yield limit for the ferrite/pearlite phase, $\sigma_{yf}$, and yield limit for the martensitic phase, $\sigma_{ym}$.

shows the thermal dilatation for specimens heated at 100°C/s and then cooled at 10°C/s (Fig. 4a), and 0.3°C/s (Fig. 4b). Both cases gave the same amount of martensitic transformation. (Here it is assumed that pure martensite is formed.) Note that the martensite start temperature, Point 2, decreases when the cooling rate is increased. This has not been accounted for in the numerical model. The thermal dilatation for reheated martensite follows the martensite curve, see Fig. 4a.

3.2. Mechanical properties

A thermo-elasto-plastic model based on von Mises theory has been used for the welding simulation using the MSC.MARC software. It is assumed that no creep strains occur during welding since the material is exposed to a high temperature for a very short period of time. However, creep is assumed to only occur during the holding sequence of the heat treatment process because of the low creep strain rate at temperatures below 500°C. This constitutive relation was also used by Josefson [11] and the assumption of independence between plastic- and creep-strain increment is supported by Otterberg [15]. The hardening behaviour of the material is assumed to be isotropic and piecewise linear. The total strain rate $\dot{\varepsilon}_{\text{tot}}$ is subdivided into elastic $\dot{\varepsilon}^e$, thermal $\dot{\varepsilon}^t$, plastic $\dot{\varepsilon}^p$, and creep $\dot{\varepsilon}^c$ strain rates, see Eq. (1).

$$\dot{\varepsilon}_{\text{tot}} = \dot{\varepsilon}^e + \dot{\varepsilon}^t + \dot{\varepsilon}^p + \dot{\varepsilon}^c.$$  (1)

Transformation plasticity is not accounted for in the model. However, other authors, for example Rammerstorfer et al. [16], have shown that transformation plasticity can be important when determining residual stresses.

The temperature dependent Young’s modulus and Poisson’s ratio are shown in Fig. 5a whilst Fig. 5b shows the virgin yield limit for the initial ferrite/pearlite mixture, $\sigma_{yf}$, and the yield limit of pure martensite, $\sigma_{ym}$.

The yield limit of the material changes due to the phase transformation from ferrite/pearlite to martensite. If the peak temperature during welding has been higher than 850°C ($A_{c3}$) the yield limit follows the curve for martensite when the material is cooled. The curve denoted $\sigma_{yf}$ in Fig. 5b is followed during cooling if the peak temperature has been lower than the $A_{c3}$-temperature.

The heat treatment simulation takes account of this peak temperature dependent yield limit and the amount of plastic deformation resulting from the welding process. To avoid convergence problems in
the numerical calculations the minimum yield limit was set to 20 MPa and the maximum Poisson’s ratio to 0.45.

The creep strain rate is modelled by applying the commonly used Norton’s law [17].

\[
\dot{\varepsilon}_{ij}^{cr} = k \bar{\sigma}^n s_{ij},
\]  

where \( \dot{\varepsilon}_{ij}^{cr} \) is the creep strain rate, \( \bar{\sigma} \) the equivalent stress and \( s_{ij} \) the deviatoric stress. The constants \( k \) and \( n \) in Eq. (2) can be determined by performing stress relaxation tests in the specific temperature interval. In the present work, Norton’s law was used with parameters obtained only at the holding temperature and only for the martensitic material, since the residual stresses generated by the welding process are highest in the area where the dominant material phase is martensite.

3.3. Thermal properties

The temperature dependent thermal properties are shown in Fig. 6a. The latent heat of melting was 338 kJ/kg. \( T_{\text{solidus}} \) was 1480 °C and \( T_{\text{liquidus}} \) was 1600 °C. The emissivity factor used for the radiation boundary condition is shown in Fig. 6b.

4. Heat input for welding

To reduce the computational time for the welding simulation an axisymmetric model was used with 1315 elements and 1862 nodes. Heat input was simulated by a moving heat source where the energy input is distributed as a double ellipsoid; a method first proposed by Goldak [18]. The parameters \( a, b, c_f \) and \( c_r \) in Fig. 7 were adjusted to create the desired melted zone. Another way to estimate the heat source parameters is to make temperature measurements on certain positions and compare these with the computed temperature field.

It is assumed that the material from the filler wire has reached melting temperature when it first comes into contact with the material surface. Because the filler material is included in the finite element mesh before the welds are performed, the elements corresponding to the filler material is treated separately. The described behaviour is simulated by giving the volume corresponding to the filler material a low yield limit and zero thermal dilatation before the temperature has reached the
melting temperature. This minimise the effect on the structure before the temperature has reached 1750 K. Thereafter, the elements are given normal properties.

The changes in material behaviour and any residual stresses and deformations due to the tack-welds have not been taken into account in the model. The heat transfer coefficient assumed for all external surfaces during and between the welding sequences was 10 W/m².

5. Heat transfer model in stress relief process

An important issue when simulating heat treatment is how well the boundary condition in the model represent the actual process. If correctly modelled, heat transfer from the surroundings should give the correct temperature gradients in the component. This section deals with the heat transfer between the component and it is surroundings inside the heat treatment furnace. The process can be divided in three different sequences, heating, holding and cooling, see Fig. 8.

Heat treatment takes place in a vacuum furnace with an operating pressure of ca 10 Pa, see Fig. 9. Even heating is achieved by the use of radiating elements located in the walls, ceiling and under the supporting grid where the component is positioned. During the cooling phase, argon gas is pumped into the charge volume from an external vessel. The gas enters through holes in the top of the furnace and passes out through holes in the bottom. The cooling gas is subsequently re-circulated on a 30 s cycle until the component reaches room temperature. The initial temperature of the cooling gas is 20 °C but is heated by the furnace walls and the components in the furnace. The gas temperature stabilises at about 60 °C after a certain time due to a heat exchanger in the furnace and then slowly falls to room temperature during the remainder of the cooling cycle. The furnace used in this study is manufactured by Schmetz and is of type MU 450/3H (150 x 1504 System 2R Futur).

5.1. Heating sequence

Knowledge about the component’s behaviour during heat treatment is important in order to understand how temperature and temperature changes affect stresses and dimensions in the final component. A high heating rate will generate temperature gradients, which could give rise to unwanted plastic strains. It is therefore important that the temperature distribution in the component is controlled.

Fig. 7. Double ellipsoid heat source.
Thermal radiation from the radiating elements on the walls of the furnace provide the heat input to the component, see Fig. 10. Heat transfer by convection can be ignored due to the low operating pressure in the evacuated chamber. The temperature of the furnace walls is monitored by a number of temperature gauges. The furnace wall temperature is controlled to follow a prescribed heating curve, see Fig. 8. The holding time is controlled by the measured temperature at certain positions near the component.

The symmetry line in the model acts as a mirror for the radiation. The Monte Carlo Method was used to calculate the so-called radiation viewfactors [19]. This calculation is made at the initialisation of the thermo-mechanical simulation. These were not updated during the analysis.
5.2. Cooling sequence

Since the heat transfer during cooling is mainly due to convective heat transfer, a fluid mechanics analysis (CFD-analysis) was performed using the FLUENT software in order to estimate the heat transfer coefficient of the component’s surfaces. This parameter is important when estimating the heat transfer between the cooling gas and the component. CFD analysis is computational demanding therefore a comparison of annular verses circular inlets/outlets was made. The aim of the study was to reduce the complexity of the model, and hence the computational time without losing too much accuracy.

The standard k-ε turbulence model, described in the FLUENT manual [20], and resolved boundary layer was used for all cases. The CFD analysis was made with a 3D-model with the boundary conditions given in Table 1.

Because of the cyclic symmetry of the furnace and component, a sector model could be used, see Fig. 11. As already mentioned, two different models, one with circular hole (Fig. 11a) and a model with annular inlets and outlets (Fig. 11b) were compared. The effective inlet/outlet area was the same in both cases.

The different inlet and outlet shapes were evaluated using data from the path shown in Fig. 12b. The heat flux along the path given by simulations with different inlet and outlet shapes is shown in Fig. 12a. The conclusion from this comparison was that the surface heat flux from the two models agrees quite closely. Since the annular inlet model is axi-symmetric, a two-dimensional model can be used, thus saving computational time.

One way of connecting the CFD- and FE-analyses of the heat treatment process is to export a parameter that describes the heat transfer between the component and gas. The heat transfer is
Table 1
Boundary conditions used for the fluid mechanics simulations

<table>
<thead>
<tr>
<th>Part of model</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall</td>
<td>Non-slip</td>
</tr>
<tr>
<td></td>
<td>Adiabatic</td>
</tr>
<tr>
<td>Component</td>
<td>Non-slip</td>
</tr>
<tr>
<td></td>
<td>Initial temperature (700^\circ C)</td>
</tr>
<tr>
<td>Gas inlet</td>
<td>Velocity—evenly distributed (18 \text{ m/s (top—one hole) and 15 m/s (bottom—two holes)})</td>
</tr>
<tr>
<td></td>
<td>Constant temperature (T = 60^\circ C)</td>
</tr>
<tr>
<td>Gas outlet</td>
<td>Pressure of (10^5) Pa</td>
</tr>
<tr>
<td>Symmetry all</td>
<td>Cyclic symmetry</td>
</tr>
</tbody>
</table>

Fig. 11. (a) Sector model with circular inlets and outlets and (b) with annular inlets and outlets.

Fig. 12. A comparison of the surface heat flux on the top surface of the hub for the two different inlet and outlet types.
The convective heat transfer process can be described by Newton’s law of cooling:

\[ \dot{q}_{\text{surface}}(x, y, z, t) = h(x, y, z, t)(T_{\text{surface}}(x, y, z, t) - T_{\infty}(x, y, z, t)). \]  

(3)

The convective heat flux, \( \dot{q}_{\text{surface}} \), is proportional to the difference between the surface and the fluid temperatures. It is convenient in the FE-analysis to have a constant \( T_{\infty} \) for the component, here called \( T_{\text{bulk}} \). If \( T_{\infty} \) is taken in the mainstream of the gas flow, a change to \( T_{\text{bulk}} \) (inlet temperature) see Fig. 13, is a small approximation because the temperature in the mainstream is almost constant between the inlet and outlet see also Eq. (4).

\[ h(x, y, z, t) = \frac{\dot{q}_{\text{surface}}(x, y, z, t)}{T_{\text{surface}}(x, y, z, t) - T_{\infty}(x, y, z, t)} \approx \frac{\dot{q}_{\text{surface}}(x, y, z, t)}{T_{\text{surface}}(x, y, z, t) - T_{\text{bulk}}}, \]  

(4)

where the convective heat flux in the CFD-analysis is calculated from Eq. (5), according to [21],

\[ \dot{q}_{\text{surface}}(x, y, z, t) = -\lambda \nabla T(x, y, z, t) \cdot \hat{n}_{\text{surface}} \text{ of the component}, \]  

(5)

where \( \lambda \) is the thermal conductivity of the gas and \( \hat{n} \) is the normal unit vector to the component's surface.

It is also assumed that the time to reach steady-state flow is short, and that the change of \( h \) over time is due to changes in the velocity gradient. This is supported by Incropera and DeWitt [21] if the gas properties are constant. A constant heat transfer coefficient for each flow direction (\( fd \)) can be used when steady-state flow has been reached, see Eq. (6).

\[ h(x, y, z, fd) = \frac{\dot{q}_{\text{surface}}(x, y, z, t)}{T_{\text{surface}}(x, y, z, t) - T_{\text{bulk}}}. \]  

(6)
Fig. 14. Calculated heat flux from the CFD-model at a single point on the hub.

Fig. 15. A schematic diagram of the coupling between the CFD- and FEM-software.

Fig. 14 shows the heat flux experienced by a given point on the hub. The spikes are associated with changes in the direction of flow and are due to turbulence. However, these disturbances only affect a short period, compared with the steady-state phase. The change in flow direction is modelled by taking the result of $h$ for a converged stationary solution in each flow direction. Note that the heat flux in Fig. 14 reduces over time because of the decreasing temperature of the component surface.

5.3. **Coupling between CFD and FEM**

The simulation was made in two stages, see Fig. 15. Firstly, the fluid flow was solved using CFD. The solution for the heat transfer coefficient was processed to give the boundary condition using Eq. (6) and then used in the thermo-mechanical finite element analysis.
The coupling was accomplished by:

(I) Solving the fluid flow problem and computing the convective heat transfer coefficient $h$ between the gas and the component using Eq. (6);

(II) applying the heat transfer coefficient from step I to the FE-model, as a boundary condition, and

(III) solving the thermo-mechanical problem.

The inclusion of the computed convective heat transfer coefficient into the finite element model was done using user-subroutines. The coupling was one-way; i.e. the deformation predicted by the FE-calculation is assumed not to affect the CFD-calculation as the deformations involved are small, about 3 mm, and thus do not affect the velocity profile.

In the FE simulation, the boundary conditions from the CFD analysis are only mapped once, at the beginning of the simulation of the cooling phase.

6. Results

The total computing time for the thermo-mechanical simulation of the welding- and heat treatment process was approximately 6.5 h using a 360 MHz SUN Ultra 60. Fig. 16 shows the distribution of the von Mises stress after welding and heat treatment. The result from the axi-symmetric model has been revolved to give a better visualisation. The maximum equivalent stress is reduced from 740 MPa to approximately 400 MPa due to heat treatment.

The stress components on top of weld C are shown in Fig. 17. The solid and dashed lines represent the stresses before and after the stress relief heat treatment, respectively. The origin is located at the centre of the weld with the inner ring is positioned to the right of the origin (positive number) and the Front support to the left. The melted zone was 6 mm measured at the top of the weld; a distance from $-3$ to $+3$ in Fig. 17. The transverse stress component is the stress perpendicular to the welding.

![Fig. 16. Effective stress distribution after welding and heat treatment.](image-url)
Fig. 17. Stress distribution before and after heat treatment on the top side of weld C. The solid line represents the result before heat treatment and the dashed lines the stress state after the annealing operation.

direction and the normal stress is the stress in the thickness direction. The most significant effect of the heat treatment is on the hoop stress component, where a tensile stress of approximately 850 MPa is changed to a compressive stress of 450 MPa.

The velocity profile of the gas during the cooling phase of the heat treatment process is shown in Fig. 18. Fig. 18a shows the cold gas entering through the inlets in the bottom of the furnace whilst Fig. 18b shows the reverse cycle where the gas enters from the top. As can be seen, the main gas stream passes around the component. When the gas enters from the bottom of the furnace (Fig. 18a), the flow from the small jets near the centre leads to a higher cooling rate for the inner ring.
The principle aim of this work was to predict the change in distance between the bearing housing and inner ring; distance \( a \) in Fig. 3a. The welding fixture used prevents the structure from expanding during the start of weld A. However, deformation is caused by all the welds. The two first welds (A and B) have the greatest effect, a shrinkage of about 0.2 mm for each weld is obtained. (i.e. negative number in Fig. 19). Welding operations C and D have only a minor effect on the final deformation.

During the heat treating process distance \( a \) increases to a maximum of approximately 2.2 mm (see Fig. 20) before returning to a value slightly less than before heat treatment, about \(-0.22\) mm, but some parts of the structure have not cooled down to room temperature. The start value in
the diagram is the residual deformation from the welding operations. The cooling part of the heat treatment process does not generate any additional plastic strains.

7. Discussion and conclusion

Simulation of welding and stress relief heat treatment of an aero engine component has been performed. The material modelling required change of property curves that accounted for temperature related phase changes. Furthermore, the modelling of the heat input could be handled by the double ellipsoid heat input model. However, the heat transfer during heat treatment required a more advanced strategy where results from a CFD-analysis were used.

The simulations revealed that welding operations A and B have the greatest effect on the final distance between the bearing housing and the inner ring. It was also found that the stress relief heat treatment reduced residual stresses to an acceptable level and reduced the shrinkage that was caused by the welding process. It was found that the cooling stage of the heat treatment process does not give rise to any additional plastic strains.

In order to obtain a more accurate result, a 3D-model of the welding process should be used. Dike [22] performed a simulation of circumference pipe weld and showed the difference in stress state was dependent on the angle from the weld start point. An axi-symmetric model cannot capture this behaviour and clearly the results from an axi-symmetric based simulation of the welding and heat treatment would not be the same as those based on a 3D-model. Using a temperature dependent creep law would also improve the simulated transient behaviour during the heat treating process. The input parameters for such a model must be obtained from creep tests carried out over a range of temperatures.

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References


Constitutive modelling and parameter optimisation
CONSTITUTIVE MODELLING AND PARAMETER OPTIMISATION

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Key words: Identification, constitutive, strain-rate jump tests, modelling, Matlab, optimisation.

Abstract. A toolbox for parameter identification has been developed using Matlab®. Different tools for optimisation are therefore readily available for the parameter determination process. There are also other useful facilities that motivated this choice of platform for the implementation. The constitutive model has been programmed using a general stress-strain algorithm so the same logic can also be used when implementing the material models into a finite element code. The used radial return approach handles models with a yield surface for which a so-called consistency condition exists and also models with a flow potential surface with a flow strength equation. The first condition states that the stress state cannot be outside the yield surface whereas the flow strength equation directly gives the plastic strain rate as a function of how far outside the flow potential surface the stress state is. The details of the numerical algorithm for the stress-strain computation are described in an accompanying paper. Different material models and methods for parameter identifications are discussed in this paper to set the general context. It focuses on the optimisation process and an application on strain rate jump tests for Greek Ascoloy is described. We present results from parameter fitting using a viscoplastic model with nonlinear, isotropic hardening. An optimisation strategy of the “divide and conquer” type was necessary to use for obtaining the seven material parameters of the chosen model.
1 INTRODUCTION

The use of finite element modelling for design of manufacturing processes is less developed than its use in design of components. This is due to the fact that these simulations are more difficult to perform because of their nonlinear character that demands both more expertise of the user and more powerful hardware and software. The hardware is becoming less of a problem for every month and there exist commercial finite element codes that have quite advanced features. Furthermore, they can be extended by means of user routines. However, the problem of modelling boundary conditions and material behaviour always remains. This paper is concerned with the latter aspect, which is crucial for a successful simulation. There exists many models to choose among but parameters are lacking. Thus an important step in finite element modelling is the material modelling stage. It consists of at least one of the steps: i) obtaining test data, ii) choosing constitutive model, iii) numerical implementation of stress calculation algorithm and iv) finding material parameters.

This paper presents a combined approach where the same numerical implementation of a constitutive model to be used in the finite element code is used in the material parameter identification process. The toolbox for parameter identification and a workbench for loading have been implemented in Matlab®. The workbench can be used for preliminary evaluation of the constitutive model and/or its numerical implementation. The use of a high-level programming language makes this prototyping very efficient. This work can then be directly used when performing the parameter identification and the Matlab® tools for optimisation are readily available. Furthermore, it is simple to port the algorithm to the finite element code when the material modelling stage is completed. This paper focuses on the Matlab® implementation and its application on Greek Ascoloy. Different material models, numerical algorithms and methods for parameter identifications are discussed to set the general context and an application of the toolbox for Greek Ascoloy is described. We present results from parameter fitting using a viscoplastic model with nonlinear, isotropic hardening. An optimisation strategy of the “divide and conquer type” was used for obtaining the seven material parameters for the chosen model.

2 CONSTITUTIVE MODELS

Constitutive models are formulated in accordance with the basic equations of thermodynamics including the equations of solid mechanics and down to the theory of plasticity. This is a subject of its own and will not be described here. The reader is referred to Malvern¹, which is an appropriate starting point giving the basic principles and constitutive equations. The book by Simo and Hughes² gives a good overview in context of plasticity and, together with the papers ³,⁴, shows one possible approach for formulating elasto-plastic relations for large deformation problems.

An additive decomposition of the strain rates is assumed. This can be motivated in different ways starting from the multiplicative decomposition of the deformation gradient, see
for example\textsuperscript{2,6}. Some of the issues in these derivations disappear when assuming small elastic strains, see Ch. 19 in 6 and Reference 7. This is reasonable for metal plasticity. Thus we have\textsuperscript{1}

\[
\dot{\epsilon} = \dot{\epsilon}^e + \dot{\epsilon}^p + \dot{\epsilon}^\theta
\]

where \(\dot{\epsilon}\) is the total strain rate, \(\dot{\epsilon}^e\) is the elastic strain rate, \(\dot{\epsilon}^p\) is the plastic strain rate and \(\dot{\epsilon}^\theta\) is the rate of the thermal strain. The latter is purely volumetric and will not be discussed in this paper. The elastic behaviour is described by a hypoelastic relation\textsuperscript{6}

\[
\dot{\sigma} = C \dot{\epsilon}^e + \frac{\partial C}{\partial T} \dot{T} \epsilon^e
\]

where \(\dot{\sigma}\) is an objective stress rate, \(T\) is temperature and \(C\) is a matrix with the elastic material properties. The updating takes place in a fixed configuration. It is furthermore assumed that the plastic strains are purely deviatoric, see for example Stouffer\textsuperscript{8}, and that the pressure does not affect the plastic deformation, i.e. deviatoric plasticity is assumed. We define a yield surface, \(f\), for which a stress state inside, \(f < 0\) or \(f = 0\) and \(\dot{f} < 0\), corresponds to an elastic deformation process. The surface is written as

\[
f = \sigma - \sigma_y
\]

where \(\sigma_y\) is called the yield limit and \(\sigma\) is the effective von Mises stress defined by

\[
\sigma = \frac{3}{2} \langle \xi \rangle \mathbf{P}_M \xi
\]

where

\[
\xi = \sigma - \alpha
\]

is the deviatoric stress, \(\sigma\), minus the backstress \(\alpha\). The latter is explained below. \(\mathbf{P}_M\) is a matrix combining the projection of stresses to the deviatoric space, the use of vector notation and the definition of the effective stress. Reference\textsuperscript{9} shows how it is used for general as well as plane stress states. Crisfield, Ch 14.6 in 6, describe how it can also accommodate anisotropic plasticity. See appendix for details about this and the matrix \(L\) introduced next.

We will use effective plastic strain rate \(\dot{\epsilon}^p\) as a measure of the magnitude of the plastic strain rates. It is defined by \(\dot{\sigma}^p = \alpha \dot{\epsilon}^p\) leading to

\[
\dot{\epsilon}^p = \sqrt{\frac{2}{3} \epsilon^p : \mathbf{L}^i \epsilon^p}
\]

where \(L\) is a diagonal matrix with the diagonal (see Ch 6.5 in 10 for details)

\[
\mathbf{L}_{\text{diag}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 1 & 2 & 2 \end{bmatrix}
\]

\textsuperscript{1} We use the so-called Voigt notation and engineering strain definition
The magnitude of the effective plastic strain rate is obtained from the so-called consistency condition for the type of models with a yield surface

\[ \dot{f} = 0 \]  

as we can never have a stress state outside the yield surface, \( f > 0 \), in this model. This is usually a rate-independent plasticity model but it is possible to include the effect of strain rate by having a rate-dependent yield surface. The magnitude of the effective plastic strain rate is obtained from the flow strength equation in the other type of models. This always gives a rate-dependent plasticity model. We will use relations where the rate is a monotonous increasing function of the excess stress \( f \) or overstress defined by Eq. (3) where we for this case can have \( f > 0 \).

\[ \tilde{\varepsilon}^p = g \left( \gamma \cdot \phi(f) \right) \]  

where the bracket \( \left\{ \right\} \) denotes that the rate is zero if \( f \leq 0 \). The introduction of \( g \), \( \gamma \) and \( \phi \) facilitates the identification with some models like those in \(^{11,12}\). These notations will be used in the discussions later. Furthermore, maximum plastic dissipation is postulated leading to associated plasticity. The yield surface is the plastic potential for the plastic strains. It gives the components of the rate of the plastic strain as

\[ \tilde{\varepsilon}^p = L^L \frac{\partial f}{\partial \sigma} = \tilde{\varepsilon}^p \frac{3}{2\sigma} L \tilde{\sigma} \]  

The hardening/softening behaviour of the material can have an isotropic and a kinematic part. The first is accounted for by the change of the yield limit of the material and the latter by translating the yield surface by changing the backstress \( \alpha \). The hardening is described by evolution equations where some examples are given in the next chapter.

The evolution equations for isotropic and hardening behaviour are discussed below and these relations can be used both for type of models. Furthermore, flow strength equations for creep and viscoplasticity are given. These general relations are illustrated by some simple examples and by the viscoplastic model applied to Greek Ascoloy in Chapter 6 and also by a model from Bammann\(^{13,14}\).

We will focus on the broad class of deviatoric plasticity models with a yield surface or a flow strength equation within the framework given above. We will not make any difference between plasticity, viscoplasticity or creep strains but only use the term plastic strains in our notations. We will not discuss temperature effects, phase changes, high strain rates and anisotropy in the discussions below.

### 2.1 Isotropic hardening

The isotropic hardening includes both hardening and recovery processes. They may be accommodated in the yield limit in yield function in Eq. (3), \( \sigma_y \), but also in viscosity, \( \gamma \), of the flow strength equation, Eq. (9). We will describe some evolution equation for the yield limit below. The initial yield limit is given as
\(\sigma_y(0) = \sigma_{y0}\)  \hspace{1cm} (11)

Its evolution equation can be written as
\[
\dot{\sigma}_y = H_{iso}\dot{\varepsilon}^p - D_{iso}\dot{\varepsilon}^p - S_{iso}
\]  \hspace{1cm} (12)

Some authors separate the equation for yield stress by introducing
\[
\kappa = \sigma_y - \sigma_{y0}(T)
\]
\[
\dot{\kappa} = H_{iso}\dot{\varepsilon}^p - D_{iso}\dot{\varepsilon}^p - S_{iso}
\]  \hspace{1cm} (13)

\(H_{iso}\) denotes hardening and \(D_{iso}\) dynamic recovery. Both are active during plastic straining. Furthermore, we have a static recovery term \(S_{iso}\). They may be functions of different parameters like effective plastic strain, or dislocation density, temperature etc. Bammann\(^\text{13}\) uses Eq’s (13) and (14) with
\[
\sigma_{y0}(T) = C_y e^{-\frac{C_i}{T}}
\]  \hspace{1cm} (15)

and
\[
H_{iso} = hG(T)
\]  \hspace{1cm} (16)

where \(h\) is a hardening parameter and \(G\) is the temperature dependent shear modulus. The dynamic recovery term is written as
\[
D_{iso} = \tau_y(T)\kappa^2 = C_y e^{-\frac{C_i}{T}}\kappa^2
\]  \hspace{1cm} (17)

and the static recovery is written as
\[
S_{iso} = \tau_y(T)\kappa^2 = C_y e^{-\frac{C_i}{T}}\kappa^2
\]  \hspace{1cm} (18)

The coefficients, \(C_y\), are material constants. Bammann \(\text{et al.}\)\(^\text{14}\) extended this equation with additional terms to account for directional changes in the loading. Most models only include the hardening term, \(H_{iso}\). Different variants of power law relations have been proposed like in the Ramberg-Osgood equation. A similar term appears in the Johnson and Cook model\(^\text{15}\). The hardening is given by
\[
\sigma_y = nK(\varepsilon^p)^{\frac{1}{n}}\dot{\varepsilon}^p \text{ or } \sigma_y = \sigma_{y0} + K(\varepsilon^p)^{n}
\]  \hspace{1cm} (19)

Another variant is\(^\text{16}\)
\[
\sigma_y = \sigma_{y0} + Q_1\varepsilon^p + Q_2\left(1 - e^{-\lambda\varepsilon^p}\right)
\]  \hspace{1cm} (20)

The last relation will be used in the parameter fitting case in this paper.
2.2 Kinematic hardening

The so-called Bauschinger is accommodated by the use of back stresses, \( \alpha \). They correspond to internal micro-stresses from pile up of dislocations and their interactions. The amount of observed kinematic hardening also depends on whether a small or large offset definition of yield is used. Kocks argues that it should be evaluated so it only includes “permanent” softening. However, modelling using a small offset definition can also be useful for some applications. The evolution equation below for kinematic hardening also includes hardening and recovery processes. The initial back stress is given as

\[
a(0) = \theta
\]

and its evolution equation can be written as

\[
\dot{\alpha} = \frac{2}{3} H_{\text{kin}} L^{-1} \kappa - \frac{2}{3} D_{\text{kin}} \dot{\sigma} \alpha - \frac{2}{3} S_{\text{kin}} \alpha
\]

where \( H_{\text{kin}} \) denotes the hardening process and \( D_{\text{kin}} \) denotes dynamic recovery. Both are assumed to be proportional to the plastic straining. The hardening term corresponds to the Prager model. It does not work directly in plane stress subspace but can be reformulated for this case, Ch 15 in 6. Furthermore, we have a static recovery term \( S_{\text{kin}} \). Bammann uses

\[
H_{\text{kin}} = \frac{3}{2} H G(T)
\]

where \( H \) is a hardening parameter. The dynamic recovery term is written as

\[
D_{\text{kin}} = R_s(T) \kappa^2 = C_{11} e^{-C_{12}/T} \kappa^2
\]

and the static recovery is written as

\[
S_{\text{kin}} = R_s(T) \kappa^2 = C_{11} e^{-C_{12}/T} \kappa^2
\]

The \( C \)'s are material coefficients. The viscoplastic relation used in this study does not include any kinematic hardening, as there were no cyclic tests available. It should be noted that the kinematic hardening could be very important for cyclic loading. It has been found that it maybe necessary to include nonlinear kinematic hardening for many cases, see for example 20-25.

2.3 Flow strength equations

The flow strength equation (Eq. 9) plays the same role as the consistency condition (Eq. 8) when determining the amount of plasticity.

The use of a flow strength equation of the form in Eq. (9) includes creep as the special case when the yield stress goes to zero. The paper by Kassner and Pérez-Prado discusses a number of relations and physical processes like dislocation glide, diffusion processes etc. leading to the specific relations in different stress-temperature domains. Frost and Ashby have
some of these discussions\textsuperscript{27,28} and several chapters in the book edited by Miller\textsuperscript{29} discuss processes and models. See also reference 8. Domkin and Lindgren apply the same tool to a dislocation density based material model\textsuperscript{30}.

The viscoplastic model used in the current study has a form that is common, a power law relation, Ch. 6.4.2 in\textsuperscript{16}.

\[
\dot{\varepsilon}^p = g(\varepsilon \cdot \phi(f)) = \left( \frac{1}{K_a} \right)^N f = \left( \frac{\sigma - \sigma_y}{K_a} \right)^N
\]  

(26)

We set (there is no a unique choice)

\[
g(\varepsilon) = \left( \frac{\sigma}{K_a} \right)^N
\]

(27)

\[
\gamma = K^{-1}
\]

(28)

\[
\phi(f) = f
\]

(29)

where \(K_a\) is a viscosity parameter and \(N_a\) is the exponent in the power law. The model used by Bammann\textsuperscript{13} represents another type of models.

\[
\dot{\varepsilon}^p = g(\varepsilon \cdot \phi(f)) = K_1 \cosh\left( \frac{\sigma - \sigma_y}{K_1} \right)
\]

(30)

We set

\[
g(\varepsilon) = K_2 \cosh(\varepsilon)
\]

(31)

\[
\gamma = K_2^{-1}
\]

(32)

\[
\phi(f) = f
\]

(33)

where the viscosity parameters are

\[
K_1 = C_1 e^{-C_1/f}
\]

(34)

and

\[
K_2 = C_2 e^{-C_2/f}
\]

(35)

The \(C\)'s are material coefficients as in the earlier chapters.

\section{STRESS-STRAIN ALGORITHMS}

The numerical solution of the constitutive relations for use in finite element simulations must be strain driven. This means that the strain is given and the stress should be computed. Furthermore, a consistent constitutive matrix is needed in order to retain the convergence properties of the Newton-Raphson method. The book by Simo and Hughes\textsuperscript{7} describes these aspects and Crisfield gives some basic numerical methods in Ch. 6 in\textsuperscript{10} and extensions in\textsuperscript{6}.  

7
Belytschko et al.\textsuperscript{31} also devote some chapters to constitutive models and stress-strain algorithms.

We use an operator-split approach where an elastic predictor is followed by a plastic corrector. We will describe it in small-deformation context as the algorithm is form-identical for large deformations if the stress updating is done in an unrotated configuration like when using the Green-Naghdi stress rate (Box 3 in 32, Ch. 19.3 in 6). We will formulate models based on yield surface or flow strength equations in parallel. A formulation can be used where the first is a sub case of the latter\textsuperscript{33,34}. We will use another approach here as it was found to be better for models with high exponents in the power law used in the flow strength equation. We follow the ideas in Ch. 15.12 in 6 and Ch 5.9.8 in 31 where the flow strength equation is solved to obtain the effective plastic strain increment. This approach is also used in References 28, 35, and 36. Details about the numerical implementation are given in the related paper, Reference 30.

\section{PARAMETER IDENTIFICATION}

Parameter identification can sometimes be straightforward as different parameters can be directly obtained from tests. However, this is not possible for models where parameters are not easy to identify directly by some features in test results. Then a systematic and objective computer based procedure for parameter identification is necessary. This is formulated as a maximisation of a likelihood function or a minimisation of an error\textsuperscript{37,38}. We use the latter approach. This error measure is minimised with respect to the material parameters. We write

Minimise \[ e(p) \mathrel{\in} \mathbb{R}^n \]  

Subject to constraints

\begin{align*}
 c^e_i(p) &= 0 & i &= 1..\text{neq} \\
 c^m_i(p) &\leq 0 & i &= 1..n_{\text{in}} \\
 \mathbf{L} &\leq p & \leq \mathbf{U}
\end{align*}

Where \( p \) is a vector with the \( n \) unknown parameters and \( e \) is an error measure. The constraints can be nonlinear equations and \( \text{neq} \) is the number of equality and \( n_{\text{in}} \) the number of inequality constraints. \( \mathbf{L} \) and \( \mathbf{U} \) are lower and upper limits for the parameters.

We consider the problem as strain driven. The strain history is given as \( n_{\text{inc}} \) number of strain increments. Bruhns and Anding\textsuperscript{38} write the error measure as

\[ e(p) = \frac{1}{2} r^T \mathbf{G} r \]  

where \( \mathbf{G} \) is a diagonal matrix with individual standard deviation errors for the measured data. The vector \( r \) has the square of the difference between computed and experimentally obtained stress \( r_i = (\sigma_i - \mathbf{\bar{\sigma}})^2 \) at different times or strains. Mahnken and Stein\textsuperscript{39} discuss the possibility of adding a regularization term to Eq. (40) in order to overcome the problem of
numerical instabilities due to non-uniqueness. They also discuss the use of the eigenvalues of the Hessian matrix in order to evaluate the robustness of the solution.

The matrix $G$ can be used also to make the error non-dimensional\textsuperscript{40} and include user defined weight functions, $w(\varepsilon)$. We use

$$G_{ii} = w_i \Delta \varepsilon_i \quad \text{no sum over } i$$

(41)

where $w_i$ is a weight factor evaluated at increment number $i$ at strain $\varepsilon_i$ associated with an interval $\Delta \varepsilon$.

A direct parameter fitting can be applied for tests where it is possible to measure over a homogenous deformed volume in order to obtain strain and stress, Figure 1a. This is the case in the current study. $p_{\text{final}}$ is the material parameters that minimize the difference between computed $\sigma$ and measured stress $\sigma_e$. A more general approach is to use an inverse modelling technique\textsuperscript{40-45} where a finite element model of the test is used, Figure 1b. $O$ is measured quantities and they are separated into loading (independent quantities), $O_l$, and experimental results (dependent quantities), $O_e$. The independent values are prescribed to the finite element model and the computed results $O_{rc}$ are compared with the measured in order to find the best material parameters.

![Diagram](image)

**Figure 1**: Parameter fitting with homogenous test giving stress and strain data (a) and with tests where inverse modelling is needed (b).

There are deterministic or stochastic methods\textsuperscript{37}. Typically some kind of gradients methods is used in the first approach. These methods can be quite efficient but finds only local minima\textsuperscript{46,47}. Thus they are very dependent on the starting value. Genetic algorithms can be considered as stochastic algorithms\textsuperscript{48,49}. They have an underlying logic of survival of the fittest but also use random generation when creating new candidates for the wanted parameters. They are quite independent on the starting values but require more iterations. Thus they can be combined with gradient methods for obtaining good starting values, Bruhns
and Anding. The system developed by Furukawa et al. combine these methods to gradient-incorporated continuous evolutionary algorithms (GICEA). Bruhns and Anding also used parallel computing to speed up the procedure. Huber and Tsakmakis used a neural network for parameter fitting.

The effect of uncertainties in the obtained stress-strain relations will also affect the subsequent evaluation of results from analyses using the obtained model. Salomonsson shows an example in the case of life time prediction.

The references above show the need for a systematic approach to parameter fitting has driven the development of software for this purpose. Furukawa et al. show some details of the user interface of their computer program. They do not use a logic for stress computation that can be implemented into finite element codes. On the other hand, their system allows the user to interactively define new material models.

5 TOOLBOX FOR MATERIAL PARAMETER IDENTIFICATION

The motivation for the development of the toolbox was described initially and the basic philosophy of using the same constitutive algorithms as for finite element computing and the underlying theory has been described shortly above. Here we only touch upon some other implemented facilities. An example of some of the user interfaces is shown in Figure 2.

The developed toolbox has modules for the following steps

- Input and processing of experimental data
- Material model selection and set up of parameter space with constraints
- Prepare optimisation by giving initial values and parameters for optimisation process

The optimisation can be started after completing these steps. It is possible to choose between a genetic algorithm or a gradient based optimisation. The first algorithm was downloaded from www.mathworks.com and the latter belongs to the Matlab® optimisation toolbox. Some facilities in the first two steps are described below.

5.1 Input and processing of experimental data

The experimental results are read in from a file. It is assumed that the strains, stresses, times and temperatures are stored column wise. The two last columns are optional. These data may be reduced, as there may be unnecessary many measurements. Furthermore, the measured data may have some scatter that can be smoothed by different smoothing options. It is possible to read data from several tests and make a parameter identification that minimises the error with respect to all tests at the same time.

5.2 Material model selection and set up of parameter space with constraints

The user can choose the material model and set initial parameters that can serve as starting values to the smoothing. The parameter used by the optimisation is normalised with respect to the initial values. Thus all initial parameters sent to the optimisation routine will be unit (1). It is also possible to change the default upper and lower bounds for all parameters. If the upper and lower bound is the same, then it is assumed that this parameter is fixed and it is not
optimised. It is possible to restart the optimisation from previous obtained values and vary the strategy of choosing to fix different parameters.

Figure 2: The main (top) together with the window in which material model and parameter range is set and windows for specifying weight function and choosing optimisation algorithm.

6 APPLICATION OF TOOLBOX FOR GREEK ASCOLOY

The results from parameter fitting using a viscoplastic model with nonlinear, isotropic hardening are presented. Greek Ascoloy, a martensitic stainless steel, is studied. The material data is acquired from strain rate jumps test, where three different strain rates are used in the same test. These tests were performed for five different temperatures and two different initial phase compositions of the material, one mixture of ferrite and pearlite and one fully martensitic. The test temperatures are 20, 600, 700, 800 and 950°C. At 800°C the material composition is assumed to be 55% austenite and the rest is the initial phase, at 950°C the material is fully austenised.

The viscoplastic model in Eq. (42) is used
\[ \dot{\varepsilon}^p = g\left( \gamma \cdot \phi(f) \right) = \left( \frac{1}{K_\alpha} f \right)^{K_\alpha} = \left( \frac{\sigma - \sigma_i}{K_\alpha} \right)^{K_\alpha} \]  

(42)

with isotropic hardening according to Eq. (43)

\[ \sigma_i = \sigma_{i,0} + Q_1 \varepsilon_p^p + Q_2 \left( 1 - e^{-\lambda\varepsilon_p^p} \right) \]  

(43)

This gives the hardening

\[ H' = Q_1 + b Q_2 e^{-\lambda\varepsilon_p^p} \]  

(44)

No kinematic hardening or recovery effects are accounted for. Thus, seven material parameters must be determined. The parameter identification procedure is discussed in Section 4. The logic for the optimisation is shown in Figure 1a.

First, we tried to estimate all parameters simultaneously by giving initial values and upper and lower bounds as constraints for them. However, this procedure was sensitive with respect to the initial guess and the optimisation did not always converge. Moreover, if the same test is performed for many temperatures, then there should be some reasonable variation with respect to temperature of the parameters. For example, the yield limit should be non-increasing with increasing temperature for the same phase. It was necessary to fix Young’s modulus and the virgin yield limit to obtain this. These parameters were possible to estimate from the initial part of the tests. Young’s modulus was assumed independent of phase composition whereas the virgin yield limit depended on the microstructure. The initial values for the hardening parameters used in the optimisation were also estimated from tests. An additional restraint was put on the hardening parameter, \( Q_1 + Q_2 b \leq E \). This means that the slope of the curve must decrease after initial yielding. The viscoplastic parameters \( N_\alpha \) and \( K_\alpha \) were comparatively less controlled than the other parameters, \( 1 \leq K_\alpha \leq 2000 \) and \( 1 \leq N_\alpha \leq 30 \). A comparison (not included here) between the measured and computed strain rate jump tests, using the parameters obtained after this initial optimisation showed a quite good fit except for the last strain rate region pass in the test. Therefore, the fitting procedure was continued with these parameters as initial guess in a fitting procedure where none of the parameters was fixed. The result from this fitting procedure is presented below.

The measured and computed strain rate jump tests are presented in Figure 3 for the mixture of ferrite and pearlite, and Figure 4 for the austenite microstructure, Figure 5 for the martensitic. In the strain rate jump test the three different strain rates were used, \( 8.3 \times 10^{-3} \text{ s}^{-1} \), 0 to 1 % strain, \( 0.6 \times 10^{-4} \text{ s}^{-1} \) 1 to 1.5 % strain, and \( 3.7 \times 10^{-6} \text{ s}^{-1} \) 1.5 to 2 % strain. The obtained virgin yield limits and Young’s modulus are presented in Figures 6a and b. The latter is independent of microstructure. The viscoplastic parameters \( N_\alpha \) and \( K_\alpha \) are presented in normalised form in Figure 7. The hardening parameters \( Q_1, Q_2, \) and \( b \) are given in Figure 8.
Lars-Erik Lindgren, Henrik Alberg and Konstantin Domkin

Figure 3: Parameter fitting for strain rate jump tests of material with initial ferrite/pearlite microstructure. Measured (circles) and computed (line) data.

Figure 4: Parameter fitting for strain rate jump tests at higher temperature when material has transformed to austenite. Measured (circles) and computed (line) data. Left figure has ferrite/pearlite and right figure has martensite as initial phases.
Figure 5: Parameter fitting for strain rate jump tests of material with initial ferrite/pearlite microstructure. Measured (circles) and computed (line) data.

Figure 6: a) Virgin yield limit. b) Young’s modulus
Figure 7: Parameter for the viscoplastic model. fp – ferrite/pearlite, m – martensite

Figure 8: Parameter for the hardening model. fp – ferrite/pearlite, m – martensite

7 CONCLUSIONS

A toolbox for parameter identification was developed using Matlab®. The toolbox was used for evaluation and fitting of parameters to the chosen constitutive model. This was a viscoplastic model with nonlinear, isotropic hardening. The following observations were made:

- The toolbox approach was an efficient way to test and evaluate constitutive models. The efficiency is due to the built-in functions like smoothing of test data, optimisation routines, facilities for plotting, and building of user-interfaces available in Matlab®.
- Flexibility in imposing other constraints than the common upper and lower limits is very useful. Here an additional restraint was applied on a combination of hardening parameters, \( Q_1 + Q_2 + b \leq E \).
- A “divide and conquer” strategy was necessary to use for the parameter fitting. Initially Young’s modulus and the virgin yield limit were fixed. These parameters were possible to estimate from the tests. This reduction of parameter space decreased the sensitivity for the choice of starting values and increased the optimisation speed. The parameters obtained in this first optimization were then used as initial parameters for the final optimization where all seven parameters were determined simultaneously.

8 REFERENCES

[15] G. Johnson and W. Cook, "A constitutive model and data for metals subjected to large strains, high strain rates and high temperatures", 541-547 (?).


9 APPENDIX

9.1 Explanation on the use of some matrices

The matrix $L$

Use of Voigt notation instead of tensor notations needs a correction in the scalar product between the stress or strain vector as for example in the case of computing the second invariant of the deviatoric stress

$$J_2 = s_i s_j = s_{11}^2 + s_{12}^2 + s_{13}^2 + 2s_{12}^2 + 2s_{13}^2 + 2s_{23}^2$$

$$J_2 = s^T L s = \begin{bmatrix} s_{11} & s_{22} & s_{33} & s_{12} & s_{13} & s_{23} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} s_{11} \\ s_{22} \\ s_{33} \\ s_{12} \\ s_{13} \\ s_{23} \end{bmatrix}$$  \hspace{1cm} (A1)

The matrix is also used when translating tensor formulas for strains to vector notation, as the engineering shear definition is two times the tensor definition. For example, computing the effective plastic strain rate using tensor and vector notation
The matrix \( P_M \) and the projection matrix \( P \)

Projection of the stresses to deviatoric stresses is done by

\[
\hat{\epsilon}_p = e^{p\top} L^{-1} e_p = \begin{bmatrix}
\hat{\epsilon}_{p1}^p \\
\hat{\epsilon}_{p2}^p \\
\hat{\epsilon}_{p3}^p \\
\hat{\gamma}_{12}^p \\
\hat{\gamma}_{13}^p \\
\hat{\gamma}_{23}^p
\end{bmatrix}
\]

\[
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/2 & 0 & 0 \\
0 & 0 & 0 & 0 & 1/2 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/2
\end{bmatrix}
\]

(A2)

The effective von Mises stress for isotropic material is computed by the use of \( L \) as shown in Eq. (A1) as we have \( \bar{\sigma} = \sqrt{\frac{3}{2} J_2} \). This gives together with Eq. (A3)

\[
\bar{\sigma} = \sqrt{\frac{3}{2} \sigma^\top s L s} = \frac{3}{2} (P\sigma)^\top L P\sigma = \frac{3}{2} \sigma^\top P^\top L P\sigma = \frac{3}{2} \sigma^\top P_M \sigma
\]

(A4)

This can be modified to accommodate anisotropic plasticity, see page 123 in Crisfield\(^6\). Ramm and Matzenmiller\(^9\) use the same notation for shells with a zero normal stress constraint.

The projection matrix has the properties

\[
P = P^2
\]

(A5)

and

\[
P s = s
\]

(A6)
Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment
Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment

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Abstract

A major concern when carrying out welding and heat treatment simulations is to accurately model material behaviour as it varies with temperature and composition. Early in the product development process, a less sophisticated material model may be suitable to compare different concepts where less accuracy in deformation and residual stress is acceptable. At later stages in the product development process, more sophisticated models may be used to obtain more accurate predictions of deformations and residual stresses. This paper presents a comparison of five different material models applied to the simulation of a combined welding and heat treatment process for a fabricated martensitic stainless steel component.

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Keywords: Welding; Heat treatment; Viscoplasticity; Plasticity; TRIP

1. Introduction

Welding and heat treatment are widely used in the aerospace industry. However, these manufacturing processes can generate unwanted stresses and deformations, a fact that has to be taken into consideration when designing or changing the sequence of manufacturing operations for a given component. Previous experience can offer some help, but costly and time consuming experiments are often required to evaluate component design, material selection, and manufacturing schedules. One way to decrease cost and reduce product development time is to use numerical simulation which can reliably predict the final properties and shape of a component based upon the manufacturing processes used. This kind of simulation can also help predict the effect of the chosen manufacturing sequence on the final component performance.

Simulation techniques for manufacturing processes are less well developed than the simulations used when designing components. This is because simulation of manufacturing processes are more difficult to perform and require more expertise from the user and more powerful hardware and software. Another
significant difficulty when carrying out manufacturing simulations is modelling of boundary conditions and material behaviour, both of which are crucial for a successful simulation.

This paper is concerned with material modelling. There are many constitutive models but these require expensive and time consuming material tests to acquire material data for the chosen constitutive model. Even given this data, it can be difficult to determine the material parameters for the chosen constitutive model. It is therefore important to choose a constitutive model that captures the behaviour of the material to the required level of accuracy, but at minimum cost. For example, during the early stages of the product development process, a less sophisticated model may be suitable to study different concepts, but with less accuracy as far as predicting, say, deformation and residual stresses. At a later stage of development, a more sophisticated model may be used to obtain more accurate results.

This paper presents a comparison of five material models for use when simulating a combined welding and heat treatment process for a martensitic stainless steel component. A key dimension was used to compare the results from the different material models. The material models that were compared are (1) rate-independent plasticity model including simplified model for phase changes described in Berglund et al. [9], (2) rate-independent plasticity including microstructure calculation, (3) rate-independent plasticity including microstructure calculation and transformation induced plasticity (TRIP), (4) rate-dependent plasticity (viscoplasticity) including microstructure calculation and (5) rate-dependent plasticity including microstructure calculation and TRIP. Two numerical methods to model creep during the heat treatment process were also compared. The heat treatment simulation included the use of computational fluid dynamics to obtain an approximation of the heat transfer coefficient of the component's surface during the cooling part of the heat treatment cycle, Berglund et al. [9].

2. Background

The finite element method (FEM) has been used since the early 1970's to predict stresses and deformations resulting from welding processes, Hibbit and Marcal [14] and Ueda et al. [26,37]. Welding simulation has been further investigated by many researchers, Goldak et al. [13], Oddy et al. [20], and Yang et al. [38] and several review articles on welding have been written, e.g. Lindgren [17–19].

Heat treatment simulations to predict the residual stresses and microstructure in a solid rail wheel have been carried out by Donzella et al. [31] amongst others. Whilst Thuvander [36] computed distortion due to quenching. However, simulation of the combined effect of welding and heat treatment are not common in the literature. Josefson [15] calculated the residual stresses after post weld heat treatment of a thin wall pipe and Wang et al. [28] simulated local post heat treatment of a pipe with different heated bands and used a power creep law when simulating the heat treatment process.

2.1. Material modelling

A major concern when simulating welding and heat treatment is being able to model the varying material behaviour. This is further complicated by temperature and rate effects and also the evolution of microstructure during the various processes, which will change the material properties in response to the thermomechanical history of the material and can cause transformation plasticity. A fully coupled thermal, metallurgical and mechanical coupling has been applied to a single pass weld by Inoue and Wang [32]. Börjesson and Lindgren [12] used phase-dependent material properties when simulating multipass welding. Rammerstorfer et al. [24] performed a thermo-elastic–plastic analysis including phase changes, transformation plasticity and creep. However, creep and transformation plasticity were not included in the same simulations. Ronda and Oliver [25] used different viscoplastic constitutive equations in welding simulations.
This work included deriving a consistent tangent matrix for each model but did not draw any conclusions as to which model was the most suitable for welding simulation.

A large number of physical processes involving varying strains, strain rates, and temperatures can lead to inelastic deformations. The range of processes potentially involved is one of the reasons for the large number of material models that have been developed; even when limiting the scope of the models to metals, Stouffer and Dame [8]. Different phenomena and models used to model plasticity are discussed by Lemaître and Chaboche [5] and Miller [6]. These models ranging from the deviatoric, ideal plasticity model using the von Mises yield condition and associated flow rule to complex sets of equations such as the MATMOD-model developed by Miller [6].

Rate independent plasticity, viscoplasticity and creep have been studied, modelled and used for many years. Many models have been proposed, some using a threshold, usually called a yield limit, to separate the elastic and the inelastic behaviour whilst others use no such threshold. Zienkiewicz and Corneau [29] used a viscoplastic constitutive model similar to the one used in this paper which set the yield limit to zero in order to model creep behaviour. They also developed a strategy for determining the time steps to be used based on stability considerations but did not include viscoplasticity and creep in the same simulation. Bodner and Partom [10,11] did not use a threshold but used the same constitutive model for viscoplasticity and stress relaxation (creep).

2.2. Heat input modelling

Another important issue when modelling both welding and heat treatment is how well the boundary conditions in the model correlate with the actual process. The heat input from the welding process was simulated in this study as a moving heat source where the energy input is distributed as a double ellipsoid; a method first proposed by Goldak et al. [13]. The thermal load in the heat treatment simulation is modelled as heat transfer from the surroundings over the boundary of the component. The amount of energy transferred depends on two major parameters; the temperature difference between the component surface and its surroundings and the heat transfer coefficient of the surface. Lind et al. [34] used computational fluid dynamics (CFD) simulations to obtain an approximate distribution of the surface heat transfer coefficient when quenching a steel cylinder in a gas cooled furnace. Berglund et al. [9] also used CFD simulations to approximate the distribution of the surface heat transfer coefficient when an aerospace component was cooled in a heat treatment furnace.

3. Welding and heat treatment of an aerospace component

The component and process studied in this work, as well as the simplifications made and the boundary condition applied on the numerical model are presented below.

The simulation presented in this paper is a part of an aerospace component called the Turbine Exhaust Case (TEC) which is a fabricated structure made of a martensitic stainless steel manufactured by Volvo Aero, Sweden. The inner part of the TEC is called the Hub, Fig. 1, and was the main focus of this work.

Simulation of the welding and heat treatment of the Hub was presented in Berglund et al. [9]. The work in the present paper concerns additional simulations on the same component using different material models and their affects on the key dimension.

The Hub is fabricated by welding two discs, the front and rear supports, between the bearing housing and inner ring. Many different manufacturing steps are involved in manufacturing the Hub is made,
however, as in the paper by Berglund et al. [9], the work presented here concentrates on the welding and heat treatment processes.

The component is welded using gas tungsten arc welding (GTAW) with additional filler material. Fabrication begins by welding the rear support, welds A and B in Figs. 1a and 2b, followed by welds C and D on the front support, Figs. 1b and 2b. Parts are first tack-welded together before the final welds are made. Any changes in material behaviour, residual stresses and deformations due to the tack-welds have not been taken into account. The component is heat treated after welding in order to reduce residual stresses.

A key dimension on the Hub is the axial distance $a$ between the bearing housing and the flange on the inner ring, Fig. 2a. Different simulations were used to investigate how the choice of material model affects the key dimension, $a$, and the residual stresses.

The finite element programme MSC.MARC [40] was used for the thermo-mechanical analyses of the welding and heat treatment. An axisymmetric model, with 1315 elements and 1862 nodes was used. The methods and boundary condition used for the welding and heat treatment simulations are the same as those used by Berglund et al. [9]. Special attention was paid to the thermal boundary condition during cooling in the heat treatment process. Heat transfer during cooling is mainly due to convective effects. A fluid mech-
anics analysis to estimate this heat transfer was performed using the finite volume based software FLUENT [39] before the thermo-mechanical analysis. Its results transferred to the model used in the FE-simulation, this procedure is also described in Berglund et al. [9].

4. Material models and properties

The material used to manufacture the component investigated in this study is a martensitic stainless steel. The material properties and models used are described below. The material model includes components for calculation of the development of microstructure during the process, and transformation induced plasticity strain (TRIP) combined with the use of elasto-plastic/viscoplastic/creep constitutive relations.

A fully coupled thermal, metallurgical and mechanical analysis of a single pass weld was made by Inoue and Wang [32]. In the present work, a so-called staggered approach was used to couple the thermal and mechanical fields as shown in Fig. 3. The thermal field is first calculated followed by the microstructural evolution and finally the mechanical quantities is determined. The geometry in the thermal analysis is updated one time step behind. Fig. 3 shows the involved variables.

A change in microstructure affects mechanical properties and also results in a volumetric transformation strain \( \varepsilon^{\text{tr}} \) and a deviatoric strain \( \varepsilon^{\text{tp}} \) (TRIP). The latter exists only if a stress field is present during the martensite phase change. A more detailed description of microstructural, mechanical and thermal properties of the material are described in subsequent sections. The effect of the thermal field and microstructural evolution on the mechanical solution are discussed later.

4.1. Microstructure evolution and its influence on material properties

The initial microstructure of the material consists of a mixture of ferrite and pearlite. The start temperature for the ferrite/pearlite to austenite transformation is 700 °C (\( A_1 \)-temperature) and the highest temperature for stable ferrite is 880 °C (\( A_3 \)-temperature). The austenite begins to transform to martensite at 250 °C (\( M_s \)) if the cooling rate is sufficiently high. It has been observed experimentally that if the cooling rate exceeds 0.4 °C/s when cooling from the austenite start temperature down to a temperature below 500 °C, the material becomes fully martensitic. The minimum cooling rate in the heat affected zone of the weld is greater then 10 °C/s in this temperature range and therefore that all austenite is assumed to transform to martensite during cooling. The calculation of austenite transformation for an arbitrary thermal history is based on the theory presented by Kirkaldy and Venugopalan [33]. The rate of transformation is described in Eq. (1), according to the expression proposed by Oddy et al. [20] for low carbon steel,

\[
\frac{dz_a(t)}{dt} = n \cdot \left( \ln \left( \frac{z_a(T)}{z_a(T) - z_s(T)} \right) \right)^{\frac{1}{c}} \cdot \left( \frac{z_a(T) - z_s(T)}{\Delta t(T)} \right).
\]

Fig. 3. Coupling between thermal field, microstructural evolution, and mechanical field. \( T \) is the temperature, \( z_a \) is the volume fraction of austenite, \( z_m \) is the volume fraction of martensite, and \( u_i \) is the displacement field.
The parameter $z_a$ is the austenite transformation rate, $z_a$ is the volume fraction of austenite, $z_{eu}$ the equilibrium phase composition, and $t$ the time. The material is fully austenised when $z_a$ is equal to one. The material consists of a mixture of ferrite and pearlite at the beginning of the simulation ($z_a = 0$). The parameter $\tau$ in Eq. (1) is temperature dependent. Oddy et al. [20] used the following expression (Eq. (2)) for low carbon steel where $s_0$, $s_e$, and $n$ are material constants.

$$\tau = \tau_0 \cdot \left( T - A_1 \right)^{-n}.$$  

The parameters used in Eq. (2) and presented in Table 1 were estimated from a dilatometric test Fig. 10. In this case, the equilibrium phase composition $z_{eu}$ varies linearly between the $A_1$- and $A_3$-temperature. The transformation rate equation is integrated explicitly and time step splitting is used if the temperature increment is too large. Austenite transformation only occurs during heating associated with the weld operation and the fraction does not decrease until the material transforms to martensite. The calculation of martensite fraction is based on Koistinen–Marburger's equation and is dependent on the maximum austenite fraction $z_{a max}$ created during heating, Eq. (3).

$$z_m = \left( 1 - e^{-b (M_s - T)} \right) \cdot z_{a max}.$$  

The material properties are calculated by assigning separate temperature dependent properties to austenite, martensite and the ferrite/pearlite mixture. However, Young's modulus, $E$, and Poisson's ratio, $\nu$, are assumed to have the same temperature dependency for all phases. The other mechanical properties are combined using linear mixing rules applied to the macroscopic material properties as used by Börjesson and Lindgren [12].

$$Y = z_{fp} Y_{fp} + z_a Y_a + z_m Y_m,$$

where $z_{fp}$ is the volume fraction of the ferrite/pearlite mixture, $z_a$ is the volume fraction of austenite and $z_m$ is the volume fraction of martensite. $Y_{fp}$ is the material property for the ferrite/pearlite mixture, $Y_a$ is the material property for austenite and $Y_m$ is the material property for martensite. The material properties computed by the mixture rule are the thermal dilatation, the yield limit and hardening parameters. Mechanical property data is presented in Section 4.3.

### 4.2. Thermal properties

The thermal properties of the material are assumed independent of the changes in the microstructure and the latent heats due to solid state transformations are neglected. Thus, the ferrite/pearlite mixture and martensitic phases are assigned the same thermal properties at lower temperatures whilst the properties at higher temperatures are those of austenite. The latent heat of melting was set to 338 kJ/kg. $T_{solidus}$ was 1480

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Austenite start temperature</td>
<td>$A_1$</td>
<td>700 °C</td>
</tr>
<tr>
<td>Austenite finish temperature</td>
<td>$A_3$</td>
<td>880 °C</td>
</tr>
<tr>
<td>Martensite start temperature</td>
<td>$M_s$</td>
<td>250 °C</td>
</tr>
<tr>
<td>Martensite finish temperature</td>
<td>$M_{end}$</td>
<td>75 °C</td>
</tr>
<tr>
<td>Rate exponent</td>
<td>$n$</td>
<td>2</td>
</tr>
<tr>
<td>Rate coefficient</td>
<td>$s_e$</td>
<td>-4</td>
</tr>
<tr>
<td>Koistinen-Marburger coefficient</td>
<td>$b'$</td>
<td>0.011</td>
</tr>
</tbody>
</table>

Table 1

Microstructure transformation data
The liquidus was 1600 °C. The emissivity factor, \( \varepsilon_{\text{rad}} \), used for the radiation boundary condition is shown in Fig. 4a and the temperature dependent heat conduction and heat capacity are shown in Fig. 4b.

### 4.3. Constitutive equations for mechanical behaviour

The constitutive equation and associated parameters are described below. Transformation induced plasticity is described in Section 4.4. The constitutive equations for finite deformation metal rate-independent plasticity and rate-dependent plasticity models used assume additive decomposition of the strain rates and the use of a hypoelastic stress–strain relation as presented in Belytschko et al. [1]

\[
\dot{e}_{ij}^{e} = \dot{e}_{ij}^{e} + \dot{e}_{ij}^{p} + \dot{e}_{ij}^{th} + \dot{e}_{ij}^{\text{tra}} + \dot{e}_{ij}^{\text{tp}},
\]

where \( \dot{e}_{ij}^{e} \) is the total strain rate, \( \dot{e}_{ij}^{e} \) the elastic strain rate, \( \dot{e}_{ij}^{p} \) the plastic strain rate, \( \dot{e}_{ij}^{th} \) the thermal strain rate, \( \dot{e}_{ij}^{\text{tra}} \) the isotropic transformation strain rate and \( \dot{e}_{ij}^{\text{tp}} \) the rate of transformation induced plasticity. In the material model used, it was assumed that there was no difference between the inelasticity resulting from rate-independent plasticity, rate-dependent plasticity, or creep and hence all these contributions are collected in the plastic strain term. The hypoelastic model and assumed additive decomposition of strain rates gives

\[
\dot{\varepsilon}_{ij} = C_{ijkl} \dot{e}_{kl}^{e} = C_{ijkl} (\dot{e}_{ij}^{e} - \dot{e}_{ij}^{h} - \dot{e}_{ij}^{th} - \dot{e}_{ij}^{\text{tra}} - \dot{e}_{ij}^{\text{tp}}),
\]

where \( C_{ijkl} \) is the elasticity tensor and \( \dot{\varepsilon}_{ij} \) is an objective stress rate. It is assumed that the plastic strains are deviatoric, i.e. \( \dot{e}_{ii} = 0 \) and the yield surface is written as

\[
f = \sigma - \sigma_y,
\]

where \( \sigma_y \) is the yield limit computed by the mixture rule in Eq. (4) and \( \sigma \) is the von Mises effective stress defined as

\[
\sigma = \sqrt{\frac{3}{2}} s_{ij} s_{ij}, \quad \text{where } s_{ij} = \sigma_{ij} - \frac{\sigma_{kk}}{3} \delta_{ij},
\]

where \( s_{ij} \) is the deviatoric stress tensor. The effective plastic strain rate, \( \dot{\varepsilon}_p \), is used as a measure of the magnitude of the plastic strain rates and is defined by \( \tau \dot{\varepsilon} = \sigma_p \dot{\varepsilon}_p \), which gives

\[
\dot{\varepsilon}_p = \frac{3}{2} \frac{\tau_{ij}}{\dot{\varepsilon}_p} \dot{\varepsilon}_p, \quad \text{and where } \tau = \int \dot{\varepsilon}_p dt.
\]

The maximum plastic dissipation is postulated which leads to the associated flow rule. The yield surface is the plastic potential for the plastic strains. This gives the components of the rate of plastic strain as
\[ \dot{e}_{ij}^p = \dot{\varepsilon}_{ij} \frac{\partial f}{\partial \sigma_{ij}} = \dot{\varepsilon}_{ij}^3 \frac{3}{2 \Delta} \sigma_{ij}, \]  

(11)

where \( \dot{\varepsilon} \) is the plastic strain-rate multiplier. The magnitude of the effective plastic strain rate is obtained from the consistency condition for the rate-independent plasticity and from the flow strength equation for rate-dependent plasticity, Eq. (12) or (15) respectively;

\[ \dot{f} \equiv 0. \]  

(12)

The flow strength equation is assumed to be a monotonous increasing function of the excess stress, Perzyna and Pęcherski [22], or overstress;

\[ \dot{\varepsilon}^p = g(\gamma \cdot \phi(f)), \]  

(13)

where \((\gamma) = \left\{ x \right\}^{\frac{1}{x}}\) is the MacAuley bracket. The viscoplastic model used in this paper follows the power law relation presented by Lemaitre and Chaboche [5]

\[ g(\gamma) = (\gamma)^\gamma, \quad \gamma = 1/K, \quad \phi(f) = f. \]  

(14)

Thus

\[ \dot{\varepsilon}^p = \left( \frac{a - \sigma_p}{K} \right)^N, \]  

(15)

where \( N \) and \( K \) are material parameters, Fig. 7, and obeying the mixture rule, Eq. (4). The hardening/softening behaviour of the material can have an isotropic and a kinematic part. The first is accounted for by the change of the materials yield limit and the latter by translating the yield surface by changing the backstress. The isotropic hardening/softening part can include both hardening and recovery processes. However, in the simulation presented here, softening, recovery effects and kinematic hardening were ignored and hence the extra terms in the derivation of the equations will be omitted. The evolution equation for the isotropic hardening was

\[ \sigma_v = \sigma_{v0} + Q_1 \tau_{ep} + Q_2 (1 - e^{-b \cdot \varepsilon}), \]  

(16)

where \( \sigma_{v0} \) is the virgin yield limit, Fig. 6b, and \( Q_1, Q_2 \) and \( b \), Fig. 8, are material parameters obeying the mixture rule, Eq. (4). This hardening model is discussed in Lemaitre and Chaboche [5]. The numerical solution of the constitutive relations for use in finite element simulations is discussed in Section 4.5.

Creep is caused by two primary mechanisms, dislocation creep caused by diffusion assisted dislocation motion and diffusion creep which is a plastic deformation due to diffusion of material, Stouffer and Dame [8]. In this paper, as discussed earlier, creep was included in the plastic strain. Two creep models were implemented and tested. The first was a special case of Eq. (15), where the yield limit and hardening, \( \sigma_v \), has been set to zero. This model is called Norton’s law and was used in Berglund et al. [9]. The parameters \( N_{creep} \) and \( K_{creep} \) have been determined by a curve fitting procedure applied to data obtained from a stress relaxation test at the holding temperature.

In the second creep model is not based on an explicit equation like Eq. (15), will be referred to as the interpolation creep model. For some temperatures three uniaxial creep tests were made at different stress levels and strain versus time was recorded. From the measured data the creep strain rate and accumulated creep strain could be obtained, Fig. 9. The piecewise-linear curves were stored in a matrix and used in the implemented interpolation creep model. The model calculates \( \varepsilon \) by linear interpolation the current creep (plastic) rate from current stress, temperature and accumulated creep (plastic) strain. The numerical implementation of this creep model is described in Section 4.5.
The material properties for the plastic, viscoplastic and creep models used in this paper are presented in Figs. 5–10. The material parameters in Figs. 6b, 7, and 8 were obtained from a parameter fitting procedure presented in Lindgren et al. [35].

In Fig. 6, the virgin yield limit is shown as a function of temperature for martensite, ferrite/pearlite, and austenite. Because of the lack of data for the austenite phase at temperatures below 950 °C, the yield limit was estimated as one fifth of the yield of ferrite/pearlite. Sjöström [41] gives data for the steel SS2134 (A Swedish steel standard). The yield strength and hardening modulus for austenite are taken as a fraction of the properties of ferrite/pearlite. To avoid convergence problems for rate-independent plasticity in the numerical simulation the minimum yield limit was set to 20 MPa.

The material parameters used in the viscoplastic model (Eqs. (15) and (16)) are presented in Figs. 7 and 8.
The thermal dilatation was calculated using mixture rule principle, Eq. (4). The parameters in the phase transformation equations were verified by comparing the calculated and measured thermal dilatation for different heating and cooling conditions and without any externally applied load. Thermal dilatation is the sum of the thermal expansion $e^\text{th}$ and the volume changes due to phase transformation $e^\text{tra}$. The calculated and measured thermal dilatation curves for a specimen heated at a rate of $100 ^\circ\text{C}/\text{s}$ and subsequently cooled at a rate of $10 ^\circ\text{C}/\text{s}$ are shown in Fig. 10. The data used for the thermal dilatation is shown in Table 2.

### 4.4. Transformation induced plasticity model

The phase transformations not only change the material’s mechanical properties but also result in a volumetric and deviatoric transformation strain. The transformation strain can be orientated if an applied
stress is present during the phase transformation because the volume differences between two phases generate microscopic internal stresses. At sufficiently high stresses, plasticity is induced in the weaker phase; this is often referred to as the Greenwood–Johnson mechanism, Leblond et al. 16. In this paper any selective orientation in the martensite created due to an external load is ignored, an assumption also used by Vincent et al. 27. This mechanism often referred to as the Magee mechanism can effect the overall shape of the body. The transformation strain is divided into a volumetric part, \( e_{\text{tra}} \), and a deviatoric part, \( e_{\text{tp}} \), when martensite transformation occurs. The latter term is often referred to as the transformation induced plasticity strain (TRIP). From experiments, it is known that TRIP-strain evolves in the direction of the deviatoric stress, \( s_{ij} \), Leblond et al. 16. The expression for TRIP-strain rate according to Leblond et al. 16 is

\[
\dot{\varepsilon}^p_{ij} = \frac{3}{2} K' \cdot h(\sigma, \sigma_i) \cdot \frac{\text{d}\Phi(z)}{\text{d}z} \cdot \hat{z} \cdot s_{ij},
\]

(17)

Desalos 42 used an experimentally developed expression for \( \Phi(z) \)

\[
\Phi(z) = z(2 - z).
\]

(18)

Eq. (17) also includes a parameter \( K' \), an analytical expression for which has been proposed by Leblond

\[
K' = \frac{1}{\sigma_{\text{fpa}}} \cdot \frac{\Delta V}{V},
\]

(19)

where \( \Delta V/V \) is the change of volume during austenite to martensite transformation and \( \sigma_{\text{fpa}} \) is the yield limit of the austenite phase. According to Leblond et al. 16, typical values for \( K' \) are between \( 50 \times 10^6 \) and \( 100 \times 10^6 \) MPa\(^{-1}\). The calculated value for the material used in this work is \( 60 \times 10^6 \) at room temperature (transformation strain is 0.006 and the yield limit of austenite is 100 MPa). The function \( h \) in Eq. (17) describes the proportionality between the applied von Mises stress and the transformation strain, Eq. (20).

\[
h(\sigma, \sigma_i) = \begin{cases} 
1 & n+1 \sigma < 0.5 \cdot \sigma_i(n+1T, \bar{\sigma}^p + \Delta \bar{\sigma}^p, z), \\
1 + 3.5 \cdot \left( \frac{n+1 \sigma}{\sigma_i(n+1T, \bar{\sigma}^p + \Delta \bar{\sigma}^p, z)} \right)^{-1} & n+1 \sigma \geq 0.5 \cdot \sigma_i(n+1T, \bar{\sigma}^p + \Delta \bar{\sigma}^p, z).
\end{cases}
\]

(20)

In order to obtain an unconditionally stable algorithm, the transformation induced plasticity term is evaluated implicitly. The deviatoric stress, \( \hat{z} \), and the function \( h \) are therefore evaluated at the end of each time step. The transformation rate \( \hat{z} \) is calculated in the middle of the increment but the amount of the new phase \( z \) is calculated in the end of the time step.

4.5. Integration of the constitutive models

The numerical solution of the constitutive relations used in finite element simulations must be strain driven. This means that the strain is given and from this, the stress can be computed. Furthermore, a consistent constitutive matrix is needed in order to ensure the convergence properties of the Newton–Raphson method. The book by Simo and Hughes 7 describes this and Crisfield 2,3 gives some examples of numerical methods applied to plasticity.
In the present work, an operator-split approach was used, where a plastic corrector follows an elastic predictor. The elasto-viscoplastic model presented here is a modified version of that described in Ponthot [23]. It has also been extended to account for TRIP and uses mixture rules to determine material properties from phase changes as done by Börjesson and Lindgren [12]. It is worth noting that Börjesson and Lindgren did not include viscoplasticity in their simulation. The fully implicit Euler scheme used here for stress–strain calculation is presented schematically in Fig. 11. This is identical to the radial return algorithm, as the trial deviatoric stress is coaxial with the final deviatoric stress. Ortiz and Popov [21] showed that the fully implicit backward Euler scheme, closed point projection scheme has good stability, even as the strain increments become large. The scheme guarantees that the consistency condition, Eq. (12), or flow strength equation, Eq. (15) are fulfilled at the end of the time step.

The Newton procedure may diverge for some values of the exponent $N$ in the viscoplastic model, Eq. (15). In this case, the bisection method is used to solve for the increment in plastic strain instead of the logic shown in Fig. 11. This part of the implementation is not shown, but the algorithm follows the same principle as that given in Heath [4] Chapter 5.2, together with the derivation used in this paper for Newton procedure.

The integration of the Norton creep model is the same as presented in Fig. 11 except for setting the yield limit and the hardening to zero. The interpolation creep model integration algorithm is presented in Fig. 12. This algorithm uses a bisection method whereby linear interpolation between the different curves given in Fig. 9 with respect to current stress, temperature, and accumulated plastic strain are used in order to obtain

![Fig. 11. A schematic representation of the plastic integration procedure.](image-url)
the current creep rate. The creep model is thus dependent on temperature, stress, accumulated creep strain and material microstructure.

In the interpolation creep model, creep is active when the temperature exceeds $T_{\text{melt}}/3$ and the effective von Mises stress is lower than 20 percent of the current yield for the viscoplastic/plastic model. The latter value was chosen in order to obtain a good fit with data obtained from stress relaxation tests. Creep and the plastic/viscoplastic models can be active at the same time. As discussed earlier, the plastic strain and the creep strain are assumed to originate from the same physical process and hence hardening due to the plastic/viscoplastic process will affect the creep rate and the creep strain will affect the hardening in the plastic/viscoplastic equations. In this paper, the creep model is not active during welding because of the short time at high temperatures.

In the heat treatment process, two different methods of applying the interpolation creep model have been compared, Fig. 13. In the first case, creep is only applied during the holding sequence, the Creep1-model, whilst in the second case the creep model was active during all stages of the heat treatment procedure, the Creep2-model. When the Creep2-model is used, the plastic/viscoplastic part of the increment is calculated before the creep strain increment in the numerical algorithm. The plastic/viscoplastic models are not active at all in the Creep1-model during the holding sequence.

5. Simulations and results

The total computing time for the thermo-mechanical simulation of the welding and heat treatment process was approximately 1.5 h using MSC.MARC on a 1.7 GHz Dell Precision 530 running Linux. The aim of this work was to predict the change in distance between the bearing housing and the inner ring; distance $a$ (called key dimension) in Fig. 2a and to predict the residual stresses after welding and after heat
treatment. In Fig. 14 the effect on $a$ due to the weld and heat treatment process for different material models is shown. Only the models which gives the minimum and maximum shrinkage together with results obtained from the model described in Berglund et al. [9] are shown. The value of $a$ after each sequence in the manufacturing chain is presented in Table 4. The last column in Table 4 is the change in $a$ before and after heat treatment ($a_{\text{cooling}} - a_{\text{weld D}}$). The residual stresses due to the five different material models are presented in Fig. 16 whilst the effect on $a$ and the residual stress using different creep models during heat treatment are presented in Figs. 17 and 18, respectively.

5.1. Presentation of used plasticity models

The following combinations of material models were evaluated in the welding simulations and also used during the heating and cooling phases of the heat treatment when the creep model denoted as Creep1 was used for the holding phase.

Rate-independent model (RI-model). In the rate independent plasticity model, no microstructure or TRIP effects were taken into account. Material properties changed due to changing microstructure as in Berglund et al. [9].

Rate-independent including microstructure calculation model (RIM-model). This model is the same as the RI-model but also includes microstructure calculation and the rule of mixture.

Rate-independent including microstructure calculation and TRIP model (RIMT-model). This model is the same as the RIM-model but also includes the TRIP calculation.

Rate-dependent including microstructure calculation model (RDM-model). The rate-dependent plasticity model includes microstructure calculations and the rule of mixture.
Rate-independent including microstructure calculation and TRIP model (RDMT-model). This model is the same as the RDM-model but also includes the TRIP calculation.

As stated earlier, no creep was accounted for during welding. The interpolation creep model was used during the holding sequence in the Creep1-model. No microstructure or TRIP calculations are needed during this phase. A short version of the above discussion is found in Table 3.

5.2. Presentation of used creep models

The comparison between the two creep models, Norton’s law and the interpolation creep model, and the different way to apply the interpolation creep model described in Section 4.3 are discussed here. The following acronyms are used. No microstructure or TRIP calculations were needed during heat treatment; i.e. no phase changes were present.

**Creep1:** The RIM-model, see above, was used during welding and during the heating and cooling sequences. The interpolation creep model, Section 4.5, was used during the holding sequence.

**Creep2:** The RIM-model was used during welding and during all stages of the heat treatment. However, during heat treatment, the RIM-model together with the interpolation creep model was used.

**Norton:** The RIM-model, see above, was used during welding and also during the heating and cooling sequences. The Norton creep model, Section 4.5, was used during the holding sequence.

5.3. Results

The change in dimension $a$ in Fig. 2a was monitored and the shrinkage after cooling of each weld and at the end of the different heat treatment phases can be seen in Table 4. The change versus time is shown in Fig. 14 for some of these cases. Those not shown are similar to the others.

During the welding process, all models show similar deformation behaviour, however, shrinkage for the RIM-model is significant larger then for the other cases, Fig. 14a. Note also the sharp change of the transient deformation during the cooling sequence in weld A and B for the R1-model. The predicted change in dimension $a$ is largest during the first two welds for all models. During the heat treatment process, distance $a$ increases to a maximum of about 2–2.4 mm and then decreases during cooling. The cooling part of the heat treatment process does not generate any additional plastic strains. It can be seen in Table 4 that the decrease in shrinkage, the last column, is similar for all the models tested.

The transverse and longitudinal residual stress after welding and after heat treatment for the different models are shown in Fig. 16a–d. The transverse stress component is the stress component perpendicular to the weld (x-direction in Fig. 15) and the longitudinal stress is the stress component in the hoop direction (z-direction in Fig. 15). The origin of the collection line is located approximately, at the centre of the weld and the data are collected along the arrow seen in Fig. 15. The width of the fusion zone was about 4.5 mm in all cases.

### Table 3

Acronyms and components included for the different material models tested

<table>
<thead>
<tr>
<th>Material model</th>
<th>Rate-independent plasticity</th>
<th>Viscoplasticity</th>
<th>Microstructure calculation</th>
<th>TRIP calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>RIm</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RIMm</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>RIMTm</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>RDMm</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
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<tr>
<td>RDMTm</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
</tr>
</tbody>
</table>

**Rate-independent including microstructure calculation and TRIP model (RDMT-model). This model is the same as the RDM-model but also includes the TRIP calculation.**
The transverse residual stress component after welding has the same distribution for all models except the RDMT-model, Fig. 16a. The somewhat skewed results for the transverse stress component are due to non-symmetric geometry. The longitudinal stress component after welding has about the same distribution, Fig. 16b. However, the models not including TRIP have a somewhat narrower zone around the peak stresses. The models in which TRIP is included have a lower stress than the models, which do not include TRIP, Fig. 16b.

The reduction in transverse and longitudinal stress after heat treatment is significant for all models. The transverse stress component after heat treatment has roughly the same distribution, but the distribution of the longitudinal stress for the RIM and RDM-models differs somewhat from the other models. The transverse stress component for the RDMT-model has not change much due to the heat treatment. The longitudinal stress component after heat treatment, the RIMT-, and RDMT-model have a zone with almost zero stress.

A comparison between the two creep models, Norton’s law and the interpolation creep model, and the different way to apply the interpolation creep model described in Section 4.5 are discussed below. The response in dimension $a$ due to the different models studied can be found in Figs. 17 and 18. The change in dimension $a$ after heat treatment is reduced by 7.5% compared to the results from the Creep2-model Fig. 17. Comparing Norton’s law and the Creep1-model, an increase of about 2.5% in $a$ after heat treatment was observed.

The effect on the residual stress can be seen in Fig. 18. The transverse component, Fig. 18a, has the same distribution and almost the same magnitude, except for some peaks in the Creep2-model. The longitudinal component, Fig. 18b, has the same or almost the same distribution for all models. However, the magnitude differs more then for the transverse stress components.

6. Discussions and conclusions

Simulation of welding and stress relief heat treatment of an aerospace component using five different material models was carried out. The simulations revealed that welding operations A and B have the

Table 4
Distance $a$ after each manufacturing operation

<table>
<thead>
<tr>
<th></th>
<th>Weld A</th>
<th>Weld B</th>
<th>Weld C</th>
<th>Weld D</th>
<th>Heating holding</th>
<th>Cooling</th>
<th>$\Delta$Cooling − $\Delta$WeldD</th>
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<tr>
<td>RIM</td>
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<td>−0.26</td>
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<td>−0.45</td>
<td>2.14</td>
<td>−0.34</td>
<td>0.11</td>
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<tr>
<td>RIMTm</td>
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<td>−0.49</td>
<td>−0.42</td>
<td>−0.44</td>
<td>2.23</td>
<td>−0.25</td>
<td>0.19</td>
</tr>
<tr>
<td>RDMm</td>
<td>−0.17</td>
<td>−0.29</td>
<td>−0.21</td>
<td>−0.24</td>
<td>2.42</td>
<td>−0.07</td>
<td>0.17</td>
</tr>
<tr>
<td>RDMTm</td>
<td>−0.20</td>
<td>−0.28</td>
<td>−0.22</td>
<td>−0.35</td>
<td>2.32</td>
<td>−0.18</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Fig. 15. The location of the data collection for the stress components.
greatest effect on the predicted final distance between the bearing housing and the inner ring for all the material models investigated. These results also agree with those obtained by Berglund et al. [9]. However, using the RDM model Weld D was also shown to have a considerable influence on the key dimension.

The sudden change in the transient shrinkage during the cooling sequence for Welds A and B observed with the RI-model is due to the low yield limit at that point in time. Since the mechanical properties of the material change when the martensite finishing temperature has been reached, a larger generated plastic strain and less shrinkage is observed with the RI-model compared with the RIM-model.

It has been found that the viscoplastic model (RDM) generates higher longitudinal and transverse stress components compared with the rate-independent (RIM) model. The model including TRIP generates lower
stresses in both stress components compared to the stresses generated by the model not including TRIP. The differences in peak stress and stress distributions in the two models including TRIP are negligible. It was found that the heat treatment process reduced residual stresses and shrinkage caused by the welding process. In Berglund et al. [9], it was found that the cooling stage of the post welding heat treatment process did not cause any additional plastic strains. This was confirmed for all models in this study. In the heat treatment simulation, it was found that the choice of creep model has only a minor effect on dimension a and the residual stresses. In this respect, the Norton creep law, which gives a result close to those from the interpolation creep model, is to be preferred since it is easier to obtain the required material data and less material testing is needed, i.e. less costly.

It can be concluded that during concept evaluation at the early stages of product development the rate-independent (RI) model can be used since it gives results which are almost as good as from the RDMT-model, but with less costly material testing to obtain material parameters.

Dike et al. [30] simulated a circumference pipe weld and showed the difference in stress state was dependent on the angle from the weld starting point. The axisymmetric model used in the present work cannot capture this behaviour. Other ongoing work will evaluate different geometric representations with a view to increasing the computational efficiency of the simulation in order to make it possible to use large models.

Acknowledgements

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References

Corrigendum to Paper III

Corrigendum to: "Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment"
Corrigendum

Corrigendum to: “Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment”

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1. Corrigendum

In the paper ‘Comparison of plastic, viscoplastic, and creep models when modelling welding and stress relief heat treatment’ by Alberg et al. [1], an error in the transformation strain model was found. The transformation strain for austenite to martensite $\Delta e_{tra}$ should have been 0.006 as defined in Table 2 in [1]. However, in [1] the term $\Delta e_{tra}$ was zero in the simulations due to omission. This has been corrected and new results are presented here. The conclusions given in [1] have not changed because of the new results and are therefore not included in this corrigendum.

2. Results

The change in dimension $a$ is presented in Table 1 after cooling of each weld and at the end of the different heat treatment sequences and the transient change in $a$ is shown in Fig. 1 for three material models, those not shown are similar to the others. Note the continuation between Fig. 1a and b and that the scales of $a$-axes in Fig. 1 have changed compared to [1]. The transverse and longitudinal residual stresses after welding and after heat treatment for the different models are shown in Fig. 2a–d. The response in dimension $a$ and residual stresses due to different creep models is found in Figs. 3 and 4, respectively. The acronyms for the models are defined in [1, Chapter 5.1]. The width of the fusion zone in [1] is about 4.5 mm, about the same width is obtained in this work.

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Fig. 1. The change in distance $a$ (a) during the four welding operations, and (b) during the stress relief heat treatment. This figure replaces Fig. 14 in [1].

Fig. 2. Residual stresses for the five material models: (a) transverse stresses after welding; (b) longitudinal stresses after welding; (c) transverse stresses after heat treatment and (d) longitudinal stresses after heat treatment. The stresses are collected along the path found in Fig. 15 in [1]. This figure replaces Fig. 16 in [1].
During the welding process, all models show similar deformation behaviour, Fig. 1a. Note the abrupt change of the transient deformation during the cooling sequence mainly in Weld A and B but also in Weld C and D for all models. The predicted change in dimension $a$ is largest during the first two welds for all models. During the heat treatment process, distance $a$ increases to a maximum of about 2.3–2.5 mm and then decreases during cooling, this is also obtained in [1]. In [1], it is found that the cooling stage of the post welding heat treatment process did not cause any additional plastic strains; this is confirmed for all models in this corrigendum.

In Table 1, small differences in deformation between the models including TRIP and the models where TRIP is omitted are found. The residual deformation in $a$ caused by Weld A gives the main difference between rate-independent models and the viscoplastic models. Additionally, note the positive residual deformation in $a$ after Weld C for all models, the almost identical residual deformation in $a$ after Weld B and C for all models, and the identical residual deformation in $a$ due to Weld D for all models. Another observation is the decreasing affect on the $a$ due to welding. Moreover, it is observed that the reduction of the shrinkage, the last column in Table 1, is similar for all the models investigated. As well, note the distribution in $a$ between all material models in Table 1; 0.08 mm after welding and 0.08 mm after heat treatment. The distribution in $a$ between the different material models is slighter than in [1] after welding and after heat treatment.

The residual transverse stresses after welding have similar distribution for all models, Fig. 2a. Comparing the transverse stresses after welding obtained here with the transverse stresses obtained in [1], it is observed that higher compressive stresses are generated for all investigated models particularly for the RIM and RDM-model where the changes from tensile to compressive stresses are significant. Observe that all
The scales of stress-axes in Fig. 2 have changed compared to [1] and that the transverse and longitudinal stresses are plotted as in Fig. 15 in [1].

The residual longitudinal stresses after welding have about the same distribution, Fig. 2b. However, noticeable is that the RI-model generates higher tensile stresses in the Heat-Affected-Zone (HAZ) than the other models. The models including TRIP have lower tensile stresses left of the weld in the HAZ but similar tensile stresses right of the weld in the HAZ than the models compared with including TRIP, Fig. 2b. The compressive stresses in the middle of the weld are similar for all models, except for the RDM-model which generates a higher compressive stress. Comparing the longitudinal stresses obtained here with those obtained in [1], it is found that the stress distribution between the different material models is smaller than in [1]. Furthermore, it is spotted that the longitudinal stresses generated here generally have larger compressible stresses in the middle of the weld especially for the RIM and RDM-model where the changes from tensile to compressive stresses are significant.

The reduction in transverse and longitudinal stresses after heat treatment is significant for all models, Fig. 2c–d. The transverse stresses after heat treatment have roughly the same distribution, except for the RI-model that has a substantial jump at \( x = 0 \), Fig. 2c. Comparing the transverse stresses after heat treatment obtained here with the transverse stresses obtained in [1] no major differences are observed. For the longitudinal stresses after heat treatment, it is observed that the RDM and RDMT-model almost no compressive stresses, Fig. 2d. Furthermore, the RI-model gives a significantly larger compressive stress and the highest tensile stress compared to the other models. Comparing the transverse stresses after heat treatment obtained here with the transverse stresses obtained in [1] no major differences are observed, except for the RI-model which generates significantly higher compressive stresses in the middle of the weld in this paper compared to [1].

A comparison between the investigated creep models, Norton’s law and the interpolation creep model described in [1, Section 4.3] are discussed below. The transient behaviour for the three investigated models are similar, however noticeable is the reduction of \( a \) for the Creep2-model in the initial part of the holding sequence, Fig. 3. Comparing the residual deformation between Creep1-model and Norton’s law a difference in \( a \) of 0.01 mm is observed and the same comparison between the Creep2-model and Norton’s law a difference in \( a \) of 0.08 mm is found. Note the difference in residual deformation, Fig. 3, between on one hand the Creep1-model and Norton’s law and on the other hand, the Creep2-model, this difference is not found in [1].

The transverse stresses, Fig. 4a, have the same distribution and almost the same magnitude, except for some peaks generated in the Norton’s law. The transverse residual stresses obtained here are similar to the corresponding transverse stresses in [1]. The longitudinal stresses, Fig. 4b, have the same magnitude for Creep1 and Creep2-model. The distribution of stresses for Norton’s law is reversed compared to the other models. Note, that the distribution between the different creep models are smaller in the transverse stress, Fig. 4a, compared to [1] and that the longitudinal residual stresses have changed significantly compared to [1] mainly for the Creep1 and Creep2-model, Fig. 4. Observe that all scales of stress-axes in Fig. 4 have changed compared to [1].

3. Discussions

The discussion in this chapter has changed some compared with the discussion in Alberg et al. [1]. However, the conclusions are the same as in [1] and will not be repeated here.

The simulations revealed that welding operations A and B have the greatest effect on the predicted final distance between the Bearing Housing and the Inner Ring for all the material models investigated. These results also agree with those obtained in [1]. The abrupt change in dimension \( a \) observed during welding is due to the volume change caused by change in microstructure (transformation of austenite to martensite)
and the greater change in $a$ for the two first welds are mainly as a result of the stronger coupling of dimension $a$ due to geometry but also due to the more flexible structure in the two first welds. Moreover, it is found that the rate-independent models generate more axial shrinkage (decrease in $a$) than the viscoplastic models and that the addition of TRIP only has minor effect on the residual deformation. For the heat treatment process, it is found that the shrinkage caused by the welding process is reduced; this confirms the result obtained in [1].

For the residual stresses, it is found that the RI-model generate higher longitudinal tensile stresses compared with the other models. The differences in peak stress in the HAZ and stress distributions between RIM and RDM-model are small for the longitudinal stresses. The last statement is also true comparing the RIMT and RDMT-model. Comparing the residual stresses after welding between this paper and [1] significant differences in the RIM and RDM-model are found. These differences are due to the omission of the term $\Delta \rho_{\text{trac}}$, because when the martensite is created in the middle of the weld compressive stresses formed due to the expansion $\Delta \rho_{\text{trac}}$. If this expansion is omitted, as in [1], these compressive stresses are not created. The less significant differences for the RIMT and RDMT-model are due to the addition of TRIP in these models. The TRIP forces the stresses to zero and the difference become less significant. The somewhat tilted stresses for the transverse stresses are due to non-symmetric geometry, this is also observed in [1]. Furthermore, it is found that the heat treatment process reduced residual stresses caused by the welding process, this confirms the result obtained in [1]. Additionally, it is found that the choice of creep model has small effects on dimension $a$ and the residual stresses, this confirms the result obtained in [1].

Reference

Comparison of an axisymmetric and a three-dimensional model for welding and stress relief heat treatment
Comparison of an axisymmetric and a three-dimensional model for welding and stress relief heat treatment

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Abstract. This work is part of a project dedicated to find accurate and reliable tools for prediction of welding and post weld heat treatment. In other parts of the project, a simulation method for combined welding and heat treatment simulations of the component was developed and different plastic/viscoplastic material models have been compared, these models included effects of phase changes. These simulations were made using an axisymmetric finite element model. The current paper presents welding and heat treatment simulations of the same aerospace component but now using a three-dimensional shell model. The results are compared with the previously used axisymmetric model. From the simulation, it can be concluded that the three-dimensional model gives better prediction of the dimension based on measurement performed but not presented here.

INTRODUCTION

This work is part of a project dedicated to find accurate and reliable tools for prediction of welding and post weld heat treatment. In the first part, Berglund et al. [1] developed a simulation method for combined welding and heat treatment simulations of an aerospace component. A novel feature was to use computational fluid dynamics to obtain an approximation of the heat transfer during the cooling phase of the heat treatment. In the second part, Alberg et al. [2] performed a comparison of plastic/viscoplastic models including effects of phase changes. These simulations were made using an axisymmetric model.

An important aspect in numerical simulation is the computational time. If an axisymmetric model can be used instead of a three-dimensional (3D) model, a reduction of the computational time is usually possible. However, the models need to be valued between computational cost and needed accuracy.

The current paper presents welding and heat treatment simulations of the same aerospace component but now using a 3D-shell model. The aim is to compare this with the previously used axisymmetric model.

BACKGROUND

In the early 1970s, Hibbitt et al. [3] used an axisymmetric model for welding and stress relief heat treatment of a disk. Hibbitt et al. [3] made comparison between measured and calculated results. Josefson [4] investigated a girth-butt welded thin walled pipe using an axisymmetric model. The paper also included a post weld heat treatment. In a series of paper written around 1990, welding simulations were carried out on a single-pass butt-welded thin-walled steel pipe. These simulations were compared with experimentally determined temperature and stress field. Shell elements were used in Jonsson et al. [6] and Lindgren et al. [7]. Karlsson et al. [8] used solid elements and Karlsson [9] used an axisymmetric model to model the welding of this pipe. All these models were compared in the paper by Josefson et al. [10]. The results from the different models [6-9] were consistent and agreed well with measurements except for the residual hoop stress at the surface of the weld. Murty et al. [12] obtained the wanted tensile residual hoop stress in the

WELDING AND HEAT TREATMENT OF AN AEROSPACE COMPONENT

The simulation presented in this paper is a part of an aerospace component called Turbine Exhaust Case (TEC) which is a fabricated structure made of a martensitic stainless steel. The TEC is manufactured by Volvo Aero Corporation. The inner part of the TEC is called the Hub, Fig. 1, and is the focus of this work. Simulation of welding and heat treatment of the Hub has been presented in Berglund et al. [1] and Alberg et al. [2]. The work in the present paper concerns additional simulations on the same component using a 3D finite elements shell model to study the affects on a ‘key dimension’ presented later and residual stresses in one of the welds.

Many different manufacturing steps are involved in manufacturing of the Hub. However, as in the paper by Berglund et al. [1] and Alberg et al. [2], the work presented here concentrates on welding and heat treatment. The Hub is fabricated by welding two discs, the Front Support and Rear Support, between the Bearing Housing and Inner Ring. The welding method is gas tungsten arc welding (GTAW) with additional filler material.

Many different manufacturing steps are involved in manufacturing of the Hub. However, as in the paper by Berglund et al. [1] and Alberg et al. [2], the work presented here concentrates on welding and heat treatment. The Hub is fabricated by welding two discs, the Front Support and Rear Support, between the Bearing Housing and Inner Ring. The welding method is gas tungsten arc welding (GTAW) with additional filler material.

FIGURE 1. Part of the Turbine Exhaust Case (TEC) V2500, a) Back view, b) Front View.

FIGURE 2. a) Cross section of the Hub showing, a) the structural parts and key dimension, a, and b) the location of the welds and the coordinate system used for all models.

Fabrication begins by welding the Rear Support, Weld A and Weld B followed by Weld C and Weld D on the Front Support, Fig. 1a-b and Fig. 2b. The parts are tack-welded together before the welds are made. A key dimension on the Hub is the axial distance a between the Bearing Housing and the Flange on the Inner Ring, Fig. 2a.

COMPUTATIONAL MODELS

This section describes the different geometrical models, material model, boundary conditions, and assumption made in the computational models. The finite element code MSC.Marc was used for all thermo-mechanical simulations.

The material model used in this paper is a rate independent isotropic plasticity model that accounts for microstructure variation and includes effect from transformation induced plasticity (TRIP). This material model was denoted RIMT in [2]. Details regarding the material model, material properties, and microstructure evolution models are found in [2].

Two geometrical models are used in this work. An axisymmetric solid model (denoted 2D) with 1315 four-node elements and 1862 nodes, Fig. 3a, also used in Berglund et al. [1] and Alberg et al. [2]. Moreover, a 3D-thick-shell element model, Fig. 3b, consisting of 35906 four-node elements and 35762 nodes.
During welding, the models have fixed displacements in the axial (z) and radial (r) direction at the Bearing Housing. During heat treatment, the models have fixed displacement in the axial direction at the Flange. These are the same mechanical boundary conditions used in Berglund et al. [1] and Alberg et al. [2] for the welding and heat treatment simulations. Furthermore, cooling by convection during and between the welding sequences is modelled by assuming a heat transfer coefficient for all exterior surfaces of 20 W·K⁻¹·m⁻². All welding is carried out in negative angular direction according to the coordinate system in Fig. 2b.

The heat input model used for the 3D-model is a moving heat source where the energy input is distributed as a double ellipsoid, Goldak [15]. The heat source has been modified for shell elements, the derivation omitted here. The parameters to the heat input model was adjusted to create the desired fusion zone. The heat is applied in every time step at the current position of the weld torch. To get an even heat distribution from the travelling heat source rather small time steps are needed. In the 2D-model, the energy input was applied letting the double ellipsoid heat source pass through the cross-section with the correct weld speed. In the 2D-model the heat is applied at the time when the cross section at 180° is passed by the weld torch in the 3D-model.

In the all models, it is assumed that the material from the filler wire has reached melting temperature when it first meets the material surface. Because the filler material is included in the finite element mesh before the welds are performed, the elements corresponding to the filler material is treated separately. In the 2D-model, the behaviour of the filler material is simulated by giving the volume corresponding to the filler material a low yield limit and zero thermal dilatation before the temperature has reached the melting temperature. This minimises the effect on the structure before the temperature has reached the melting temperature. Thereafter, the elements are given material properties corresponding to the current temperature. In the 3D-model the elements regarded as filler material is first activated in the thermally. When the temperature is below the melting temperature the elements are activated mechanically and are then given the mechanical properties corresponding to the current temperature. Simulation of tack welds in the 3D-model is made by activation of several elements along the weld paths. The material in the tack-welds is assumed to consist of martensite. The rest of the component consists of a mixture of ferrite/pearlite. Tack-welds were not used in Berglund et al. [1] or Alberg et al. [2] as they used an axisymmetric model. The residual stresses and deformations due to the tack-welds are not included only their effect on the stiffness. The cooling time between the welds is 500 seconds. The component is heat treated after welding in order to reduce residual stresses.

During the heating sequence in the heat treatment, the component is heated by thermal radiation as described in Berglund et al. [1]. In the 2D-model, Berglund et al. [1] calculated the thermal radiation from the furnace walls using viewfactors. However, this is not supported for shell elements in Marc. Therefore, the heat transfer by radiation in the 3D-model is modelled by Equation (1) for all exterior surfaces.

\[
q_{\text{rad}} = h_{\text{rad}} (T_{\text{surface}} - T_{\text{amb}}) \quad (1)
\]

\[
h_{\text{rad}} = \varepsilon \sigma \frac{T_{\text{surface}}^4}{T_{\text{amb}}^4 + T_{\text{surface}}^4} \quad (2)
\]

Hence, the directional properties of radiative heat transfer are not accounted for. In Equation (1), \( q_{\text{rad}} \) is the radiative heat flux, \( h_{\text{rad}} \) is the heat transfer coefficient for radiation defined in Equation (2), \( T_{\text{surface}} \) is the temperature of the component, \( T_{\text{amb}} \) is the ambient temperature in this case the temperature of the wall, \( \varepsilon \) the emissivity of the components surfaces as in Alberg et al. [2], and \( \sigma \) is Stefan-Boltzmann’s constant.

A thermal analysis of the heating sequence was made in order to compare the differences in temperature between the 3D-model and the 2D-model due to the omission of viewfactors. This investigation showed that the difference was not more than ±5% for the points investigated.
In Berglund et al. [1], special attention is paid to the thermal boundary condition during the cooling sequence of the heat treatment process. The heat transfer during the cooling is mainly due to convective effects. Therefore, a fluid dynamics analysis to estimate heat transfer coefficients was performed. This is described in detail in Berglund et al. [1]. In the 2D-model, the convective heat transfer coefficient was changed every 30 seconds due to reversal of the gas flow in the furnace, Berglund et al. [1]. The time for the cooling sequence during heat treatment is 15000 s. In the 2D-model, 500 increments was used for the cooling sequence to get the correct cooling rate due to gas reversal. In order to decrease the computational time for the 3D-model an approximation was made. The convective heat transfer coefficient used during the cooling sequence was taken as the average of the heat transfer coefficients of each gas flow direction. Since no additional plastic strain was introduced by the cooling sequence during heat treatment on the 2D-model, [1][2], this simplification seems acceptable.

SIMULATIONS AND RESULTS

The total weld length was about 4900 mm and process time for welding and heat treatment was 31058 s. The simulation was made on a Dell Precision 530, 1.7GHz, running Linux. Additionally, for the 2D-model 1 CPU was used and 3D-model 2 CPUs were used.

<table>
<thead>
<tr>
<th>Model</th>
<th>Increments</th>
<th>Computational time [h]</th>
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</thead>
<tbody>
<tr>
<td>2D</td>
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<td>1.5</td>
</tr>
<tr>
<td>3D</td>
<td>2361</td>
<td>1169</td>
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</table>

The computational time and the number of increments used in the simulations are presented in Table 1. The aim of this work is to predict the change in distance between the Bearing Housing and the Inner Ring (distance \(a\)) in Fig. 2a and compare the result between an 2D-model and a 3D-model after welding and after heat treatment. In addition, residual stresses in Weld A are compared after welding and after heat treatment, Fig. 6a-d.

The magnitude of \(a\) after each sequence in the manufacturing chain is presented in Table 2. The last column in Table 2 is the change in \(a\) before and after heat treatment \((\Delta a_{\text{cooling}}=a_{\text{cooling}}-a_{\text{weld}})\). The transient behaviour of distance \(a\) due to welding and heat treatment is shown in Fig. 4 and Fig. 5, respectively. In Fig. 4 and Fig. 5 an average magnitude of \(a\) is used for the 3D-model. The average of \(a\) is calculated from the value at the position 0°, 45°, 90°…315°. Weld A and Weld B give the largest change in \(a\) during welding for both models, Fig. 4. After the completion of the welding, it is observed that the shrinkage in the 3D-model is almost two times larger then for the 2D-model, Table 2.

During heat treatment, the same behaviour is found for both models except for the cooling sequence, Fig. 5. The different behaviour between the 2D-model and the 3D-model can be explained by the difference in heat transfer coefficient. This difference was discussed earlier in the paper. No additional plastic strain was created during the heat treatment for any model. Notice the increase in \(a\) by 0.20 mm for the 2D-model where the 3D-model increases only 0.12 mm due to heat treatment, Table 2.
The 3D-model shows the same behaviour as the 2D-model in the transverse stress Fig. 6a. However, the 3D-model has lower compressive stress negative to the weld than the 2D-model, Fig 6a. The change in sign for the 3D-model seems to be due to mesh density at the different sides of the weld. This difference in density gives a temperature difference which during cooling after Weld A give an uneven distribution of TRIP-strain which causes the sudden change in stress at \( x = 2 \text{mm} \). The difference in mesh density can be found in Fig. 6a-d, where the nodes are shown as markers. For the longitudinal stress, the 3D-model shows similarity in the distribution and magnitude compared with the 2D-model, Fig. 6b. The difference in longitudinal stress in positive \( x \)-direction seems to be TRIP-strain as discussed for the transverse stress.

The residual stresses after heat treatment have considerable smaller magnitude then after welding, Fig. 6c-d. The transverse residual stress for the 3D-model is different in distribution compared with the 2D-model, Fig. 6c. Some similarity is found between the 3D-model and the 2D-model in the longitudinal stress particularly for negative \( x \), Fig. 6d.

<table>
<thead>
<tr>
<th>Model</th>
<th>Weld A</th>
<th>Weld B</th>
<th>Weld C</th>
<th>Weld D</th>
<th>Heating Holding</th>
<th>Cooling</th>
<th>( \Delta \text{coating - coating D} )</th>
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<td>-0.41</td>
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<td>-0.41</td>
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</tbody>
</table>

**FIGURE 6.** Residual stresses for the different models. a) Transverse stress component after welding. b) Longitudinal stress component after welding. c) Transverse stress component after heat treatment. d) Longitudinal stress component after heat treatment. Data collected in 180° from weld start using the coordinate system in Alberg et al. [2], Fig. 15.
DISCUSSIONS AND CONCLUSIONS

Simulation of welding and heat treatment of an aerospace component is carried out using a three dimensional shell model and an axisymmetric solid model. The simulations revealed that Weld A and Weld B have the greatest influents on the predicted final distance between the Bearing Housing and Inner Ring for the two investigated models. These results agree with those obtained in Berglund et al. [1] and Alberg et al. [2]. It is found that the three dimensional model gives a larger shrinkage than the axisymmetric model after the welding. The reduction of shrinkage due to heat treatment is larger for the axisymmetric model than for the three dimensional model. Moreover, is found that the stresses after welding and after heat treatment have roughly the same distribution. The differences in stress is mainly due to differences in mesh density which give different temperature field which implies difference in TRIP-strain during cooling after welding.

It is found that the heat treatment process reduced residual stresses and shrinkage caused by the welding process for both models. In Berglund et al. [1] and Alberg et al. [2], it was found that the cooling stage of the heat treatment process did not cause any additional plastic strains. This was confirmed for all models in this work.

It can be concluded that the three-dimensional model give better prediction of the dimension $a$ based on measurement performed but not presented here. No conclusions regarding the accuracy of the stresses can be made since no such measurements have been carried out.

ACKNOWLEDGMENTS

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A two stage approach for validation of welding and heat treatment models used in product development
A two stage approach for the validation of welding and heat treatment models used in product development

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Many components used in the aerospace industry have complex shape and are manufactured from high strength materials. Performing large scale tests is costly and time consuming, therefore, simulation tools are needed to support an effective product development process. Using manufacturing simulations during product development requires a validated model of the material and manufacturing process. In this paper, a validation scheme is proposed for thermomechanical models of welding and post-weld heat treatment. The scheme was investigated by comparing simulations using shell elements with experimental results, which showed good agreement when predicting residual stresses after welding, but an overestimation of the out-of-plane deformations when simulating both welding and heat treatment. However, the simulations showed that the out-of-plane deformation is strongly influenced by the initial geometry. It can be concluded that the simulation model is adequately accurate to be used in concept evaluation.

Keywords: Simulation, Welding, Post-weld heat treatment, Validation, Martensitic stainless steel

Introduction

The finite element method (FEM) is frequently used by design engineers to evaluate characteristics of a product including deformations, stresses, strength, stiffness, vibration and fatigue analysis, etc. The tools used for this kind of analysis are well developed, but generally do not account for the effects of the manufacturing process. The increasing pressure to decrease product development time has led to the need for efficient tools to predict not only the behaviour of the finished product, but also the effect of the manufacturing process on the final shape. Modelling the process which is used to manufacture a component even allows service life predictions to be made, based on the residual stresses from manufacturing in combination with the stresses from in service loads.

A number of issues have to be dealt with when developing tools to support the evaluation of manufacturing effects on a product, including design and manufacturing methodology, through to constitutive relations and numerical algorithms. The effects of manufacturing processes are often complex and include non-linear phenomena, which mean that any simulation the model developed has to be validated before it is used in a design situation. The validation of manufacturing simulations at a full scale component level should be minimised because of the cost involved and limited time available.

In this paper, a validation strategy for a welding and post-weld heat treatment model is presented. This validation strategy is limited to thermomechanical models of welding and does not include welding phenomena such as weld pool geometry, microstructural development or grain boundary liquation. The validation strategy can be performed at a very early stage of product development, or, even before the work on a specific product has started, which will reduce the time needed when simulations are used at the later stages of the development cycle (Fig. 1).

The expression ‘validation’ has different meanings, depending on the research field in question. The validation as used in this paper concerns the comparison of simulation results with the behaviour of the real system to ensure that the underlying algorithms and data accurately capture the essence of the associated physics.1

Product development can be divided into a number of phases (Fig. 1).2 Manufacturing simulation can be used as a tool to link design and manufacturing during the development, for design and manufacturing engineers to evaluate different concepts or manufacturing processes. The validation of simulation models of manufacturing processes has to be carried out before the tool can be used as a ‘qualified’ tool in product development. The validation should initially be performed at a subsystem level. This is because of the cost and time involved in finding errors in a model covering a large scale or very complex and interrelated process.

The main objective of the present work was to find suitable models to be used during the concept design
phase, and to develop an approach, which could be used for the validation of thermomechanical models in general. The work indicates that good results can be achieved using residual stresses and distortions for the validation of welding and heat treatment models.

Background

In this section, different validation approaches and the mechanical problems for the computability of non-linear solid are discussed. References to welding phenomena is also made, which are not covered in detail in this paper but regularly investigated in literature, e.g. weld pool geometry, grain growth in the fusion zone, microstructural development in the heat affected zone and grain boundary liquation, etc. Zacharia et al. outlined four principle areas of welding modelling: heat and fluid flow, heat source–metal interaction, weld solidification microstructures and phase transformation. A review of the state of the art in these areas gives suggestion for the further research presented.

The validation of thermomechanical simulation models of welding and heat treatment can be performed in numerous ways depending on the specific application and the use of the results. For example, in a sheet metal forming application, the deformation of the product and reaction forces in fixtures are of interest when developing the manufacturing process associated with a particular product design. The deformed configuration is represented by the surface, the outline is the initial geometry. The weld is located in the centre of the dense mesh along the plate. In a sheet metal forming application, the deformation of the product and reaction forces in fixtures are of interest when developing the manufacturing process associated with a particular product design. In the same application, stresses and strains are of interest if the risk of cracking during the manufacturing is to be avoided, or the operating fatigue life of the product is to be estimated. However, it is important that the validation process captures the physics associated with the process, irrespective of the use. The techniques, which isolate certain phenomena, are often used when validating simulation models. Oberkampf and Trucano described a validation process for a computer fluid dynamics problem, which is decomposed into three steps: subsystem cases, benchmark cases and unit problems. Defining the subsystem involves decomposing the complete system into a manageable parts where only a limited number of the physical processes are involved. In a mechanical analysis, for example, this could involve identifying parts of the system which experience typical conditions for the complete model. An example of a subsystem case for the validation of welding is the plate shown in Fig. 2. When carrying out the decomposition, it is of great importance that the cases chosen characterise the phenomena, associated with the process being simulated, and that the subsystem effectively reveals every weakness in the model. Benchmark cases involve the isolation of a limited number of physical processes, for example, special hardware or test fixtures may be fabricated to represent the main features of each subsystem. The number of physical processes involved should be less than the number of processes in the subsystem case. One example of a benchmark case is the so called Satoh test. In a Satoh test, a test piece is clamped at both ends of a test rig, and then heated and subsequently cooled. The reaction forces can be recorded during the thermal cycle and used to validate the model. This is one of the strategies used in this paper and will be discussed in detail later. Unit problems are used for evaluation of mathematical models covering one or a few physical phenomena. An example of a unit problem is the simulation of a tensile test made to evaluate the chosen material model.

A number of different measurement techniques, many of which were mentioned by Lindgren, can be used when validating welding and heat treatment. One way of comparing the result from a computational model with the behaviour of the real component is to use deformation patterns at certain points or measurements of the component’s shape after each process step. While such a comparison gives information about the quality of the simulation, it does not give any helpful information as to where errors occur if the simulation does not agree with reality. Measurements of residual strain give more information than residual deformations because the rigid body motion is not measured and the area where
the error occurs can be more easily identified. The residual stresses of welded or heat treated structures can be measured, for example, by hole drilling, surface contour measurement, neutron diffraction or X-ray diffraction.9-11 It is important to note that acceptable agreement of the residual stresses does not necessarily guarantee that the deformation results will be good as was shown by Stone et al.9 Measurements of forces in fixtures can be used in the case of welding, but not for heat treatment where fixtures are seldom used.12 Whether a model can be considered validated or not depends on the required or adequate accuracy. Sudnik et al.13 defined an adequate model as follows: The necessary simulation accuracy must be defined on the basis of compromise between complexity and accuracy of the physical-mathematical model. Such an optimised model is termed an adequate model. The accuracy required varies, depending on whether the model is to be used at the early stages of product development or at a later stages when, for example, detailed planning of a manufacturing process is involved. At the conceptual design stage, different design and manufacturing concepts are compared and evaluated. The accuracy required for the simulation tool need to be sufficient to allow the quantitative comparison of different design concepts, in order to select the best candidates for further evaluation. On the other hand, when specifying manufacturing process parameters at the later stages of product development, the simulation results must accurately predict the magnitude of any deformations to ensure that tolerance requirements are fulfilled.

The quality of the result obtained is also coupled to the type of case studied. Belytschko and Mish defined the expression computability, which refers to how well a physical process can be computed and identified three major barriers for computability in a solid mechanics: material model and data, smoothness and stability.1

Smoothness is best understood in terms of non-smoothness or roughness in a model such as that would be seen in contact impact phenomena where the load and boundary condition changes abruptly. Welding and heat treatment models are generally smooth problems because no contact impact occurs during the process. However, stability problems such as buckling during welding or heat treatment analysis, which are non-smooth, can occur. Deo et al. showed an example involving buckling distortion of a welded T-joint configuration owing to generated residual stresses during welding.14 Predicting the final shape of a structure is difficult if buckling occurs because a small change in boundary conditions, load or initial geometry can have large influence on the deformation behaviour and final shape, and makes the validation process more complex.

Problem definition

During the earlier work, the need for an effective validation procedure was discovered.15-16 The present paper therefore aims to give answers to the following questions, which are important to the development of a validation procedure:

(i) For a simulation model of welding and heat treatment, what validation steps are necessary to be accepted as a qualified tool in the product development of aerospace components?

(ii) What phenomena or conditions should be included in the simulation models to generate adequate results?

(iii) In which situations would the simulation models be applicable on a full scale component?

(iv) Is the validation method chosen robust enough to enable the quantification of the discrepancy between measured and calculated results?

In the current work, the validation of the effects of any geometric simplification was seen to be important because the simulation model uses shell elements, which is the technique used in later, full scale component analysis. Thus, the evaluation of the validation procedure is summed up in the following question: can the final shape of a welded and heat treated test plate be predicted with the adequate accuracy using a shell model for the geometry, a double ellipsoid heat source as weld heat input model, and a thermo-elastoplastic/viscoplastic material model?

To answer this question, a subsystem and benchmark case is proposed which uses deformation and residual stress as validation parameters. Each process has its own validation steps for the material models using suitable tests that cover the relevant temperature and time range for the process. Furthermore, a simple geometry was used to validate the thermal boundary conditions for models that were uncertain.

An important foundation in the proposed validation strategy is that a validated model with appropriate material model(s), boundary conditions and discretisation in time and space can be directly applied to the full scale application. Therefore, no validation of the full scale application should be needed. Using the proposed subsystem and benchmark case, the first validation steps can be performed early in the design phase when the material and welding process are chosen, and then applied on the detailed geometry when the welding procedures are being determined (Fig. 1). The experiments performed for the validation used components taken from industry and conditions similar to those used in full scale production.

The simulation model used for the validation cases is typical of that used in the early stages of product development. In this case, adequate accuracy represents the accuracy required for concept evaluation. Important quantities to be evaluated include deformations and residual stresses after welding and the final shape after post-weld heat treatment. The residual stresses after heat treatment are not validated but can be of interest if the results are to be used for fatigue life predictions.

A deductive approach has been used when no new material models or numerical algorithms have been proposed or developed. The simulations were performed using the standard FEM codes together with commonly used material models.9

Welding process

The most common welding processes in the aerospace industry are gas tungsten arc welding (GTAW), electron beam welding (EBW), laser welding and friction welding. In this paper, it is the GTAW process that is of interest. The FEM software MARC was used for all thermomechanical simulations.17
Process and equipment

In the GTAW process, heat is produced by an electric arc between a non-consumable tungsten electrode and the workpiece. An inert gas such as argon or helium is used as a shielding gas to prevent oxidation in the weld zone. Filler material can be used and would typically be added from the side or in front of the fusion zone. Gas tungsten welding is the best suitable for welding materials with a thickness between 0.5 mm and 3 mm.

Simulation model of welding process

FEM has been used to predict stresses and deformations owing to welding since the early 1970s. Although initially used in the nuclear power industry, it is now commonly used by aerospace manufacturing companies. The use of three dimensional weld models started in the middle of the 1980s and gave more accurate deformation results than two dimensional models.

There are many examples in the literature. Roberts et al. used FEM simulations to develop a process model for EBW that predicted the residual stresses and distortion with acceptable accuracy. The prediction of deformation and residual stresses using solid or shell element models started with models of pipes in the late 1980s.

A mesh is used to represent component geometry in simulations. The level of the mesh used depends on the thickness, boundary condition and accuracy of results required, etc. In the present work, a model with 4-node thick shell element was used, where the stresses in the thickness direction were assumed to be zero (plane stress condition) and the total strain varied linearly through the thickness. The temperature distribution through the thickness was assumed quadratic and 11 layers for the numerical integration in the thickness direction were used.

The heat input in the simulation model was represented by a travelling heat source with the energy input distributed as a double ellipsoid, a model proposed by Goldak et al. The energy input in this case is distributed on the top surface of the plate. The GTAW test set-up used arc length control, i.e. the voltage between the workpiece and the electrode was kept constant by keeping the distance between the electrode and component constant. This was also used in the numerical model of the welding process. The dimensions of the heat source were evaluated on the top and bottom of the plate 20 mm from the start of the weld, and process heat source parameters were adjusted in the numerical model to obtain the same size of fusion zone as on the test plate. This procedure was not presented in the current paper. The power and efficiency were kept constant during welding and were assumed independent of geometric deformations such as changes in gap or the misalignment between the plates.

Activating elements were used to imitate the joining of material. One row of elements along the weld path was initially deactivated in the analysis. The deactivated elements do not contribute to the stiffness matrix but are active in the thermal part of the simulation. The volume of the inactivated elements corresponds to the amount of filler material added during the welding sequence. The elements were activated in the mechanical part of the simulation when the temperature matched the melting temperature and the temperature was decreasing, i.e. when the material solidified.

The material used in this study was a martensitic stainless steel and the material models included components for the calculation of phase evolution and transformation induced plasticity (TRIP) combined with the use of thermo-elastoplastic/viscoplastic constitutive relations. The material models used in this paper are denoted RIT-, RIMT-, and RDMT model as in the paper by Alberg and Berglund. Note that only the RIMT model is used during the simulation of welding. A description of the material model and material data used in this paper can be found in Ref. 15.

Stress relief heat treatment

Post-weld heat treatment is performed to obtain specific microstructures or phases and/or to reduce residual stresses owing to welding. Reduction of residual stresses was the main objective in the present work and the process is therefore referred to as ‘stress relief heat treatment’. In the aerospace industry, gas cooled vacuum furnaces are commonly used for stress relief heat treatment. In the following section, the process is described briefly and a heat transfer model is presented.

Process and furnace type

The heat treatment process can be divided into three different stages: heating, holding and cooling (Fig. 4a). Heat treatment takes place in a vacuum furnace with an operating pressure of about 10 Pa (Fig. 3). Even heating is achieved by the use of radiating elements located in the walls, ceiling and under the supporting grid, on which the component is positioned. During the cooling phase, argon gas is pumped into the chamber from an external vessel. The gas enters through holes in the top of the furnace and passes out through holes in the bottom. The cooling gas is recirculated on a 30 s cycle until the component reaches room temperature. The initial temperature of the cooling gas is 20°C but is heated by the furnace walls and components in the furnace and reaches a stable temperature of about 60°C after a time.
Simulation model of heat treatment

Detailed simulations of heat treatment processes have been carried out before, for example, Donzella et al.\textsuperscript{27} predicted the residual stresses and phases in a solid rail wheel. Thuvander’s simulation of a steel tool die showed a good correlation with measured deformation results. The prediction of the deformation of an aerospace component during stress relief heat treatment has been presented by the authors in earlier papers.\textsuperscript{15–16}

An important issue when simulating heat treatment is how well the boundary condition in the model represents the actual process, i.e. if correctly modelled, heat transfer to/from the surroundings should give the correct temperature gradients in the component. The thermal radiation from the radiating elements on the walls of the furnace provides the heat input to the component. The heat transfer by convection can be ignored owing to the low operating pressure in the evacuated chamber. The temperature of the furnace was measured by a number of thermocouples positioned at the top and bottom of the charge volume. The power input to the heating elements was controlled so as to follow a prescribed temperature curve, a closed loop control system adjusting the input power to obtain the desired temperature profile (Fig. 4). The thermocouples used in the control system are protected using a ceramic envelope illustrated in Fig. 5, which result in a lower heating and cooling rate than on the surface of the inner walls. In the numerical model, the temperature of the walls was used as a boundary condition. In Figure 5a, the simulated thermocouple and wall temperature is shown as a function of time. The thermocouple temperature represents the control temperature in the furnace and depends on heat treatment cycle. A large difference in temperatures between the wall and the thermocouple can be seen, which is due to the nature of radiant heat transfer. The wall temperature was estimated using inverse modelling of a separate local model, which is not the approach used by Berglund et al.\textsuperscript{16} The local model consists of the furnace wall and the ceramic envelope surrounding the thermocouple (Fig. 5b). The analysis of heat transfer between the wall and the envelope was started by guessing a temperature history for the wall. The temperature inside the ceramic envelope represents the temperature measured by the thermocouple. Because the guessed temperature history for the furnace wall does not generate the process input temperature inside the envelope, a new updated wall temperature was guessed (Fig. 4). The revised temperature history of the wall was updated until the temperature response inside the envelope was the same as the process input temperature.

The thermal boundary condition used during the heating sequence was used during the holding sequence, but during cooling convection boundary conditions were applied, simulating heat transfer between the cooling gas and the component. Berglund et al.\textsuperscript{16} used CFD-calculations to estimate heat transfer coefficient when modelling a full scale component, which showed no plastic strain generated during the cooling sequence. In the present work, a heat transfer coefficient of 100 W m\textsuperscript{2} K\textsuperscript{1}) was used on the top and bottom of the plate. The behaviour was assumed quasi-static and large deformations were accounted for in the same way as for the welding simulation.

To account for the creep, during the heat treatment a creep model was used. The creep model used is that proposed by Alberg and Berglund\textsuperscript{15} and is denoted Creep2-model.

Validation approach

This chapter describes the validation process for welding and postweld heat treatment, the benchmark and subsystem cases, measurement techniques and the measured quantities.
The validation of the welding and postweld heat treatment processes was divided into two cases: a benchmark case and a subsystem case, following the definition given by Oberkampf and Trucano. In the benchmark case, the material model was validated using test pieces and well known boundary conditions. In the subsystem case, the thermal boundary conditions and process parameters were validated; this step was referred to as the process validation step.

The results from the benchmark case were validated quantitatively and were independent of the stage in the product development process in which they would be used. In the subsystem case, the validation was made qualitatively by a graphical comparison and the required ‘adequate accuracy’ corresponded to a model used in the concept evaluation stage (Fig. 1). The transient deformation behaviour during the cooling sequence of welding was compared qualitatively against measurements while the residual stress owing to welding was compared quantitatively, because the stress field is an important initial condition in the heat treatment analysis.

**Benchmark cases—validation of chosen material model**

A modified Satoh test was used to recreate a temperature and stress cycle similar to that seen under welding conditions, i.e. the benchmark case for welding. Additionally, a relaxation test was used to validate creep effects under the conditions similar to stress relief heat treatment, i.e. the benchmark case for post-weld heat treatment.

A Gleeble machine was used to perform the test, as it was able to control the temperature history, stress and/or stroke with acceptable accuracy. Test specimens were used when validating the material models and the tests were performed using two geometrically different specimens. The tensile tests performed to obtain material data for the simulation models should not be considered part of the validation procedure.

**Satoh test**

The test specimens used were rods with threaded ends and, in this case, with a reduced diameter over a reference length which was necessary to obtain a homogenous temperature field through the thickness of the rod. One of the specimens is shown in Fig. 6a.

In the original Satoh test, both ends of the specimens were clamped, the rod was then heated and subsequently cooled. The specimen was heated by the current and the heat input was controlled by measuring the temperature at a reference point on the thinner part of the specimen (Fig. 6b). The transient reaction force at one end of the rod was recorded during the thermal cycle. The transient stress state obtained from this was then used as a validation parameter in the benchmark case. The Satoh test used in this work was modified somewhat. Instead of using completely fixed clamps as in the original Satoh test, controlled displacement of one of the clamps was used in order to obtain the stable force response seen in the Gleeble machine. The magnitude of the displacement rate was controlled to give the strain rate history (Fig. 7).

The axisymmetric model used in the numerical analysis is shown in Fig. 6c; note the symmetry lines. The heating cycle was simulated by controlling the temperature on the thinner part of the model and during cooling a convective boundary condition was applied on the outer part of the specimen. The controlled displacement condition was applied by a contact condition between the specimen and a rigid disc.

**Relaxation test**

In the relaxation test, a compression test performed using cylindrical test specimen with a length of 7 mm and a diameter of 5 mm. The specimen was only held in place by the compression force from the jaws. Temperature, force and the change of diameter were recorded during the test and the radial strain, calculated from the change in diameter divided by the original diameter, used as the validation parameter. A graphite foil was used to reduce the friction between the ends of the specimens and the jaws, and therefore, the friction between the jaws and the specimen were neglected in the numerical model. The material was exposed to a varying compression loads during a given temperature cycle. The temperature was varied according to Fig. 8, in three temperature steps. When the holding temperature was reached at \( T_{\text{hold1}} \), \( T_{\text{hold2}} \) and \( T_{\text{max}} \), the temperature was...
kept constant for a given time. The load was chosen as a fraction of the yield limit at each holding point. Each load step was applied before the temperature was increased to the next level. The load shown in Fig. 8 is a compressive load.

Subsystem cases—validation of processes

The aim of process validation is to check boundary conditions, loads and model discretisation for each process. The processes investigated in this work are welding and post-weld heat treatment. Process validation for welding was carried out using a fixture, which allowed large deformations during the butt welding of the plates. In the process validation step, the simulated shape of the test plate was compared with experimental results after welding and after heat treatment. The same test plate geometry (190 x 100 x 1.7 mm when welded) was used when validating both processes.

Figure 9 shows the validation parameters for the two processes and the corresponding measured quantities. The heat input in the simulation of the welding process was modelled as a travelling heat source and calibrated using the dimension of the fusion zone described earlier in this paper. This method gave temperatures very close to the measured temperatures in the paper by Lundback et al.29 The heat parameters could also be calibrated by measurements of the temperature close to the weld seam; but this technique was not used in the current work.30

Comparison of the measured and calculated transient temperature field is not a necessary condition for a valid model, because the heat input model is adjusted to fulfil certain criteria, for example, the dimension of the fusion zone during welding. However, the deviation between the temperature field used in the model and the actual temperature will be seen if the transient and residual deformations are used as validation parameters because the driving force for deformation during welding and heat treatment is the temperature. Using the size of the fusion zone and heat affected zone to calibrate the model can be an effective approach for use in the aerospace industry because these dimensions are also a qualification parameters used for process control.

Deformation was used as validation parameter to validate welding and heat treatment while for the welding process, the transient and residual deformations were used and in the heat treatment process the residual deformation was used. It is an advantage to measure the transient deformation because transient measurements give a greater opportunity to detect where the model is good and where it is weak. In this work, the transient and residual deformations were measured using an optical system on a reference area on the test plate, the optical apparatus used and the measurements presented later. Measurements of the deformations give information about the quality of the geometrical model and the level of discretisation. The transient deformation measurement during heat treatment is a complex task owing to the hostile environment in the heat treatment furnace and the problem of getting a good optical view of the reference area of the component during heat treatment.

The validation of the residual stress field after welding is important because the residual stress state represents ‘the load’ in the heat treatment analysis. In this case, the residual stresses were measured by the hole drilling

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<th>Validation parameter</th>
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<td>Residual deformation</td>
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method. For the heat treatment process, the surface temperature of the component was used as a validation parameter together with the residual deformation as described earlier (Fig. 9).

Procedure for deformation and stress measurement

Three different testing procedures were used in the experiments, but with the same process parameters for all cases. In all cases, the samples were clamped in a fixture during the welding operation and the post-welding heat treatment.

Procedure 1: one plate was engraved with a reference pattern before the welding operation and the transient deformation of the reference area were recorded.

Procedure 2: the plates, without reference pattern, were welded, heat treated, and the shape of the top surface post process measured using optical techniques.

Procedure 3: four plates with no engraved pattern were welded, and residual stress measurements made.

The aim of procedure 1 was to obtain information about the transient deformation behaviour outside the heat affected zone. The reference pattern was engraved before welding and only outside the fusion zone. The optical measurement technique used for post process evaluation is described later. The initial geometry of the plates was measured when the plates had been mounted in the welding fixture and the transient deformation measurements started when the welding procedure had finished, some 75 s after the start of the welding.

The initial shape of plates used in procedure 2 was measured when they had been mounted in the welding fixture. The shape of the specimen was measured using an optical system, some measured 600 s after the start of the welding process. Post-weld heat treatment was performed in a gas cooled vacuum furnace with the plates positioned where the cooling rate was low. The final shape was measured with the plates reassembled in the welding fixture.

A residual stress measurement using the hole drilling method was used to validate the stress state after welding. The plates used in this test were welded using the same process parameters and fixture/clamping as used in procedures 1 and 2. The residual stress was measured at the points indicated in Fig. 11 with the plates assembled in the fixture.

Experimental set-up used during deformation and residual stress measurement

The experimental set-up was designed to obtain large deformations. The plates were fixed as a cantilever beam to enable the observation of the gap and bending behaviour during and after the welding process (Fig. 11). The two plate halves were clamped without any gap and the clamping force was applied via a 20 mm thick steel plate held in place by two screws. The plates were held in position by supports on each side to minimise any deformation behind the clamping area. Gas tungsten arc welding with arc length control was used to join the plates. Pulsed current with a nominal power of 720 W was used and the welding speed was set to 2.9 mm s$^{-1}$. Argon was used as shielding gas on both the top and the bottom surfaces of the plate.

11 Dimension of the test plate used for validation
The transient deformation of a limited area was measured using ARAMIS, an optical system manufactured by GOM mbH. The system's CCD cameras were positioned above the fixture at a distance of \( y = 500 \text{ mm} \) from the reference area. The experimental set-up can be seen in Fig. 10, together with the welding robot. Note that in Fig. 10 the optical system is positioned only 200 mm from the test plate. The optical system requires a clearly visible pattern, either random or regular in nature, on the surface of the component to be measured. During welding, the surface finish changed owing to the effects of temperature. The reference pattern used was therefore created using laser engraving. The pattern used was a checkerboard of 1 mm \( \times \) 1 mm squares. The edges of the squares were engraved to a depth of \( y = 10 \text{ mm} \). The information about transient deformation cannot be obtained in the fusion zone during and after welding because the material in the fusion zone melts and destroys the etched pattern. Figure 11 shows the schematic drawing of the engraved area on the top (welding side) of the plate.

The hole drilling method was used to measure the residual stresses owing to the welding process. The residual stresses were measured at six positions 60 mm from the clamping area, and the theory for ‘blind holes’ used together with the coefficients presented by Aoh and Wei for a thin plate.\(^{30}\) The drilling was performed incrementally to a depth of 0.85 mm, which corresponds to half the thickness of the plate. The positions of the strain gauges used are shown in Fig. 11 (On the topside of the plate.) Gauge number one was positioned in the centre of the weld joint and used as reference when positioning the other gauges.

During heat treatment, the welded plate was put in a basket and positioned in the furnace where the rate of cooling was low. The residual deformation and strain after post-weld heat treatment was measured with the test piece remounted in the welding fixture.

**Temperature validation during heat treatment**

Heat transfer during heat treatment is mainly owing to radiation and therefore on the emissivity of the component and surrounding surfaces. During the cooling, heat transfer is strongly depending on the velocity of the cooling gas, the geometry of the component and its surroundings. The validation of the heat transfer between the walls of the furnace, cooling gas and the workpiece has to be performed using actual geometry owing to the major influence of the geometry on the process. One way of validating the temperature is to use existing charge elements and to position these at ‘extreme’ locations in the furnace, i.e. where the heat transfer is assumed very high or very low. These tests were not performed in the work presented here.

**Comparison of measurements and computations**

This paper presents a road map for the validation of simulation models used for welding and post-weld heat treatment. The validation process should be performed before the simulation tool is used in actual product development to minimise errors and to estimate the potential and accuracy of the simulation model. The results of the material validation are shown in the next section for the Satoh and relaxation tests. Thereafter, the result from the process validation is given, together with a discussion of the influence of important properties. The effect of the initial shape of the test plate and the modelling of the yield limit of the molten material are also investigated.

**Validation of material model**

The result from the Satoh test and the relaxation test are presented in this section. The experimental and simulated result from the Satoh test with a heating rate of \( 323.15 \text{ K s}^{-1} \) and a cooling rate of \( 293.15 \text{ K s}^{-1} \) are shown in Fig. 12. In the simulations, three different material models are compared: the RIM-, RIMT- and RDMT models.\(^{15}\) The measured stress is calculated by dividing the reaction force \( F \) (Fig. 12), with the initial area in the thin section of the specimen. It can be seen that the RDMT model gives a higher compressive stress during heating and a lower tensile stress during cooling compared with other models and the experimental measurements. The difference between the results...
obtained with the three material models is mainly due to viscoplasticity. The lack in the agreement between the material models and the measurements between \(700^\circ C\) and \(1100^\circ C\) during cooling is due to a jump in the measurements, which is caused by backlash in the Gleeble machine. During cooling, martensitic transformation starts at \(250^\circ C\). The lack in agreement for the RI model is because of the omission of TRIP strain in this model. Comparisons of RIMT- and RDMT model results with experimental data show that \(M_s\) is set too low in the phase evolution model. The difference between RIMT- and RDMT models is due to a slightly different implementation of the TRIP strain calculation. Among the investigated material models, RIMT model seems to give the best agreement with the experimental results.

In the relaxation test, the change of diameter was used as validation parameter. The measured and calculated results are presented in Fig. 13. The temperature and diametrical change were measured in the middle of the specimen and the applied force at each temperature level chosen to obtain a stress level of 90% of the yield limit at each temperature. A thermo-viscoplastic (creep) model was used and no phase transformations were assumed to occur during this process owing to the temperature. The creep model gives quite good agreement at 550 °C and 700 °C, however, the simulated creep rate at 650 °C is higher than that of the measured result. The lower creep rate in the creep model has to be investigated further.

Validation of welding model
In this section, the measured results are compared with the calculated results from the welding tests. As stated earlier, the validation of the welding process is by comparison of computed and measured residual stresses, deformations and transient deformations (Fig. 9). During the residual stress measurements, the test plates were clamped in the welding fixture at room temperature. The stresses were compared along an imaginary line in the \(y\)-direction passing through strain gauges 1–6 (Fig. 11). The calculated residual stresses are presented in Fig. 14 together with the measured results achieved by the hole drilling method. The \(x\)-axis in Fig. 14 represents the distance from the centre of the weld, i.e. zero is in the middle of the melted zone. The stresses are almost symmetric around the weld centre and the stress component in the longitudinal direction is shown on the left side of the figure. The stress in the \(y\)-direction, perpendicular to the weld, is shown on the right side (positive distance). The error bars show the variations between the measurements for four different plates. Good agreement can be seen between the measured and calculated residual stresses as shown in Fig. 14. The discontinuities seen in the residual stress are due to the rather coarse mesh used in the melted and heat affected zones (0–10 mm). The coarseness of the mesh can not cope with the large stress gradients in these areas.

The simulated and measured out-of-plane deformation is shown in Fig. 16. The measured residual deformations after welding show a large variation between the plates. In some cases, the out-of-plane deformation is in different direction although the weld and fixturing are the same. The residual mismatch along the weld also varies between plates. Figure 15 shows the measured out-of-plane deformation of two welded plates: test 1 and test 2. The deformation can be seen to be asymmetric around the weld path in test 1 (Fig. 15a) and significant misalignment between the individual plates can also be observed. This can be due to initial misalignment, which was larger in test 1 than in test 2. No investigation regarding these differences has been made although the
Factors such as the alignment of the samples with respect to the direction of rolling of the sheet from which they were cut could be significant. The initial shape of the plates in test 2 was measured and used in the simulation and a comparison with measurement after welding and after heat treatment made.

Figure 16 shows the measured and simulated out-of-plane deformation after welding (test 2). A positive value represents a deformation upwards and the isoline for an amplitude of 3.4 mm is shown in the result from the simulation model. The maximum out-of-plane deformation in the model is 5.5 mm and the maximum measured is 3.4 mm. The relatively poor correlation of the out-of-plane bending results could be due to several effects and has to be investigated further. In the weld model a constraint is applied to guarantee a smooth transition between the individual plates and the initial geometry was acquired from measurement. The constraint forces the same out-of-plane displacement between the nodes in the weld seam. Without the constraint, a large mismatch is seen during the welding simulation. This model is referred to as weld model 1 (WM1).

The transient deformation during welding was measured over a reference area using the optical system. Measurements started 43 s after the welding and continued for 500 s. The initial shape of the reference area was used as a reference state and the deformation was calculated from the reference configuration. Figure 17a shows the measured deformation in the y-direction for one of the test plates. Because of oxidation, no information about the deformation in the heat affected zone could be obtained. The transient y-deformation and final gap in the front of the plate are similar in all experiments. The measured and calculated y-deformation at a single point (shown in Fig. 11) is given in Fig. 17b. The experimental curve starts at 75 s after and the y-displacement decays during the cooling sequence and becomes ∼0.1 mm 300 s after welding starts. No simulation of the same initial geometry was carried out owing to the lack of information about the initial geometry of this plate.

The yield limit of the molten material has a significant effect on the magnitude of the computed y-deformation and is illustrated by the results shown in Fig. 17b. A simulation model using a yield limit $\sigma_{\text{ymin}}$ of 20 MPa gives a larger y-displacement than the model using a 5 MPa yield limit. The magnitude of the result obtained in the simulation is higher than the experimental values and the y-deformation can be seen to stabilise at a certain level. This is not the case in the experiments. Attempts to use a yield limit for the molten material of less than 5 MPa, lead to simulations that did not converge or errors such as non-positive definite system of equations.

The influence of the initial geometry on the out-of-plane deformation was investigated by the welding simulations. The investigation was made by giving the WM1-model an initial ‘butterfly’ deformation. Weld model 2 (WM2) was given a butterfly angle of 1° and weld model 3 (WM3) a butterfly angle of -1°. The definition of the angle is shown in Fig. 18 together with the residual out-of-plane deformation of the sampling point. The residual deformation is in opposite directions for WM2 and WM3. The final deformation result shown in Fig. 18 can be seen to be sensitive to the initial geometry.

The use of shell elements instead of more general solid elements reduces the size of the model. A comparison of these techniques is given in the report of Berglund et al.\textsuperscript{31} While shell elements can not reproduce the stress field near the weld, the current work shows a good agreement between measured residual and computed stresses as seen in Fig. 14. This was also found by other
researchers, for example, Lindgren and Karlsson performed welding simulation of a butt welded pipe using shell elements. A comparison between shell, solid and axisymmetric discretisation for welding simulation of the pipe used in the report from Lindgren et al. is presented by Josefson et al. The error in deformation shown in Fig. 16 seems to be due to effects other than the discretisation used.

**Validation of heat treatment simulation**

The measured and calculated out-of-plane deformations during the post-weld heat treatment are presented in Fig. 19. The magnitude of the measured deformation is larger than in the model, but the deformation behaviour is similar. The negative sign of the deformation represents a downward bend. The disagreement in the out-of-plane deformation might be due to the disagreement for the welding (Fig. 16), however this problem has to be investigated further.

**Discussion and conclusions**

This paper presents a validation strategy for welding and post-weld heat treatment models. A ‘qualified’ simulation tool is necessary to assure the quality of simulation result when used in product development. The proposed validation process can be carried out at the predevelopment phase when the material and manufacturing procedures are known (Fig. 1).

The validation process presented is divided into two steps: material and process validation. Decomposing the validation process in this way has the advantage of ‘qualifying’ the material model before the process is simulated. The focus of the process validation step (subsystem case) is then on the loads and boundary conditions in the process. Material and process validation has to be performed whenever a new material is to be qualified because the dynamics of the welding arc and the flow in the melted zone are not simulated. The weld process model is therefore only valid for a particular weld groove geometry and process parameters. Similar mesh density and time steps to those used in the validation case have to be used when analysing the full scale component to ensure that discretisation errors are not increased in the simulation of the full scale component.

Whether the model can be considered as valid depends on the scope of subsequent simulations on full scale components. If the scope is to estimate the residual stresses owing to welding, the current model can be considered valid since the distribution of the stresses and the maximum amplitude show good correlation between the model and experiments. It can therefore be concluded that the discretisation using shell elements gives valid results for residual stresses.

The situation is different if distortion is of importance. If validation weld parameters are used on a full scale component, there is a large risk of buckling unless this is prevented by fixturing and/or tack welds. It is therefore important to know the initial deformation and depending on the required accuracy of the deformation results, the model can be valid or not. The model is probably accurate enough to be used in concept evaluation because the deformation behaviour can be predicted if the initial geometry is known. However, it is not accurate enough to predict the gap or the mismatch in front of the weld because the material behaviour in the weld pool cannot be modelled with sufficient accuracy.

The validation subsystem represents an extreme case because the geometry is allowed to move in almost all directions during welding. The deformation behaviour is easier to predict if the component is tack welded and/or if clamping is used to reduce the degree of freedom more than in the validation model. In this case, the accuracy of the current model could be adequate when used for detailed analysis. The behaviour of the fixturing of the subsystem should reflect the conditions expected with the full scale component and if tack welds are present in the component model, they should also be included in the validation model. No conclusions can be given regarding the discretisation owing to the problem of buckling.

There is always a risk associated with using a structure or process that is sensitive to input parameters (process parameters, geometry and material data) because large differences in the results can occur as shown with the initial ‘butterfly’ angle. The robustness of the subsystem used for validation presented in this paper can be questioned because of the large deviations observed between experiments which depend on material, geometry and process parameters. The deformation predicted during the subsystem validation can be instable and reveals the instability of the process, which, together with the parameters mentioned above, can give large differences in deformation result.

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Berglund et al. Validation of thermo-mechanical models

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