Neural network modelling of submerged arc weld metal properties

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Neural Network Modelling
of Submerged Arc
Weld Metal Properties

By
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A doctoral thesis submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy

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Abstract

There are many problems in welding metallurgy for which it is difficult to develop a first principles scientific model due to their complexity. A significant problem faced by today’s welding engineers, is the need to relate welding parameters to the quality of the finished weld. This is usually done by experience, and the need for many experimental trials, eventually leading to optimal welding parameters. Important characteristics in the evaluation of line-pipe seam weld quality are the weld bead shape and size, which can have a significant effect on the microstructure and mechanical properties of the weldment through heat flow effects. Properties of the final weld may therefore be difficult to predict, especially quantities such as weld metal toughness, which are known to be dependent on many factors. One approach to such complex problems is to use neural networks. A neural network is an artificial simulation of the brain which models data through a learning process and stores the information as a set of rules akin to knowledge. This research is concerned with the application of neural network techniques to the prediction of the mechanical and physical properties, including the shape of the weld bead, of submerged arc line-pipe steel welds.

A limited experimental investigation has been carried out using optical and transmission electron microscopy to establish an understanding of the complex microstructures that result from the welding processes used in the production of line-pipe. Particular attention was paid to the role of complex inclusions in the nucleation of acicular ferrite, the dominant phase in such welds.

The main focus of this work is the prediction of a number of useful weld parameters. The starting point of any weld model is to determine the final chemistry of the weld bead, which is a function of both plate, wire, and flux chemistry. A multiple output neural network model has been developed to enable prediction of the complete weld metal chemistry, which is a significant improvement on previous work. This is then further developed and applied to the prediction of weld metal toughness, a notoriously difficult quantity to determine through physical models. Similar approaches have been successfully used to model other difficult phenomena such as the tendency for hydrogen induced cracking to occur.

A model has been developed which can predict the complete shape of an entire asymmetric weld bead with great accuracy. Initial approaches considered only the outer diameter weld bead,
Abstract

whereas later developments were able to additionally incorporate the inner diameter bead. Great care has been taken in this work in choosing appropriate inputs and architectures for the neural network models, and attention has also been paid to the relevance of the various inputs in contributing to the outputs. Novel methods of digitisation of weld metal macrostructures made under different experimental conditions, used in training of the neural network, are considered.

In summary, a complete approach to the determination of weld metal phenomena has been discussed. The ability to predict an entire weld bead shape is extremely useful and it is now possible to use this as an input into ‘through process’ models for the entire welding process.
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Chapter 1 - Introduction

1.1 Thesis Overview

Submerged arc welding (SAW) has become the manufacturing method generally preferred in the production of large diameter steel line pipe. This is due to the high productivity achieved to a consistent standard. However, one significant problem faced by today's welding engineers, is the need to relate welding parameters to the quality of the finished weld. This is usually done through experience, and requires many experimental trials, eventually leading to optimal welding parameters. The aim of using SAW is to produce high quality welds at low cost, and therefore an efficient method for the determination of weld quality in order to optimise welding practices is required.

Mechanical properties, such as toughness and ultimate tensile strength (UTS), being key characteristics used in the evaluation of weld quality, can vary greatly in weldments due to the changes in the metallurgical structure during the fusion process. These properties are affected by the weld chemical composition, weld bead shape, volume, area of heat-affected zone (HAZ), plate type and heat input. Although modelling of these mechanical properties has been achieved using a variety of techniques\(^1\)\(^-\)\(^5\), certain areas of the weld and welding process are omitted due to assumptions in modelling or simplifications made. Therefore, a suitable method for predicting the weld bead shape from process parameters is needed as a fundamental base for predicting dependent mechanical properties. Examples of areas where this could be further applied are the modelling of heat flow and strain distortion within the weld, with the ultimate aim being a 'through process' model.

Even though physical models based on the fundamental principles have become increasingly sophisticated and can account for several of the mechanisms that influence weld shape, they are still not useful for most production applications. These model types usually require many computer hours to run, being far too slow for real time simulations. More recent models have made use of neural network models, enabling prediction of situations too complex for simpler multiple linear regression techniques. Neural networks can be considered as a powerful means of non-linear regression analysis and pattern recognition, with wide ranging applications. These methods can be used widely in materials applications, especially when matching large numbers
of variables with one or more dependent outcomes. Neural networks have been proven as a useful tool in the optimisation of many processes including welding, in which the relationship between manufacturing parameters and the weld bead shape is not a simple one, due to the high number of competing variables.

In the work presented within this thesis, a neural network approach within a Bayesian framework using Markov chain Monte Carlo methods has been taken to predict weld metal chemistry, mechanical properties and weld bead shape for 3 wire one pass per side submerged arc welds. The overall aim of the project is to deliver a series of models enabling prediction of weld metal chemistry, weld metal properties and weld bead geometry from a knowledge of plate and wire type and welding process parameters.

1.2 Formation of Line-pipe

Several processes are involved in the production of a tubular structure from a flat sheet of steel prior to the welding process, including inspection steps after each stage to ensure a good quality pipe; the full process is highlighted in a video by Europipe of Germany, and on the website of SAW pipes, Texas, USA. The process employed at the pipe mill in Hartlepool, UK, is known as the U-O-E process, standing for U-ing, O-ing and expansion. This method is employed due to the large diameter of pipe being manufactured; other possible methods are the J-C-O process for medium to large diameter pipe, and seamless processing for small diameter pipe.

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\textsuperscript {Def.1} Bayesian framework; the weights and biases of the neural network are assumed to be random variables with specified distributions. The regularisation parameters are related to the unknown variables associated with these distributions. We can then estimate these parameters using statistical methods.

\textsuperscript {Def.2} Markov chain Monte Carlo (MCMC) methods provide a way of numerically computing the integrals required to obtain posterior distributions in the neural network, this works by simulating the posterior. A Markov chain is constructed whose equilibrium distribution is the posterior we want. A large number of samples are taken from the chain (say, 500) to allow the chain to reach equilibrium.
1.2.1 Pre-Welding Processes

Prior to formation of the pipe the steel plate undergoes inspection. Inspectors receive, identify and examine mill-certified plates in the plate-receiving bay. They identify plates by heat number and assign each a unique pipe serial number that is marked on the pipe and permanently recorded. Following this the plate is sent for edge milling; automatic rollers convey the plate to the edge miller, which mills the plate to the precise width and bevels it for longitudinal welding. Continuous monitoring ensures accurately planed edges. Milled plates proceed to the crimping press, which curves up the longitudinal edges, beginning the formation into pipe. A two-stage process is employed in the shaping of the flat plate to the “O” shaped vessel. Firstly the plate goes through a U-ing process, as seen in Figure 1.1(a). The hydraulic U-press shapes each crimped plate into a symmetrical “U”, before being moved onto the O-ing phase, as seen in Figure 1.1(b). Hydraulic presses up to 28,000 tons bend the “U”-ed pipe into a complete circle, and then the O-shaped form is ready for welding.

1.2.2 Welding

There are 3 stages of welding undertaken in the manufacture of line-pipe; these stages are tack welding, inner diameter (ID) welding and outer diameter (OD) welding. Tack and tab welding is a vital preparatory step that helps prevent many causes of weld defects, such as burn-through and cracks. The tack weld will later be completely consumed by the subsequent SAW welds made at the ID and OD of the pipe as illustrated in Figure 1.2. Tabs, welded onto each end of the pipe, ensure proper lead-in and run-off of the weld during automatic welding operations. Tack welds can be continuous or intermittent dependent upon the specifications set out for the line-pipe specification.
The ID and OD welding processes are fully automated ensuring good consistency. 4-wire submerged arc welding machines produce a continuous bead from tab to tab along the internal seam of the pipe, shown in Figure 1.1(c). Welding parameters are closely controlled to pre-set values throughout ID and OD welding, and the flux is kept moisture-free to ensure high-integrity
welds. Quality Control personnel inspect the pipe, and then it is conveyed to the OD welder for continuous tab-to-tab outside diameter welding using a multiple wire submerged arc-welding process. An example of a 3-wire submerged-arc welder being used in the OD welding of line pipe can be seen in Figure 1.1(d).

![Diagram highlighting the position of welds applied to the line pipe material, showing in particular the position of the tack weld consumed by both Id and OD welds](image)

**Figure 1.2** – Diagram highlighting the position of welds applied to the line pipe material, showing in particular the position of the tack weld consumed by both Id and OD welds

1.2.3 **Mechanical Expansion**

After pressure washing to remove loose mill scale the pipe is mechanically expanded. The expansion ratio for a 42-inch pipe is normally in the range of 0.8% to 1.5%. This improves its properties and ensures the dimensional integrity of the finished product. Mechanical expansion to true roundness reduces residual stresses and achieves uniform diameters, making the pipe easier to join and weld in the field, this can be seen in Figure 1.1(e).
1.1 Modelling of Materials and Industrial Processes.

A model can be described as a concise description of a body of data, or a simplification of the real phenomena that occur in nature. Science has evolved through modelling nature and simplifying things where it is necessary. At best a model captures the essential physics of a problem, highlighting the principles that support the key observations and can predict behaviour under conditions that have not yet been studied. Transformation of inputs into outputs is key to the formation of a successful model, which may take the form of algebraic, differential, or integral equations, and these may be embedded in a discretised computation. Therefore, in summary, a model is firstly a simplified description of a system, and secondly the formalisation of this system in a mathematical way.

Models can be very complex mathematically even with a very simplified description of the process to be modelled. Often the resulting equation systems are analytically insoluble requiring further simplifications of the model for a solution to be reached. However, computers may be able to provide an exact numerical solution in some cases through the ability to carry out a high number of calculations or iterative processes at high speed. Computer modelling is the implementation of a model in a computer system, for example through the use of computer code. Once a model is implemented in the computer, the system can be simulated. Computer simulations are the study of the responses of a modelled system by a given choice of inputs that simulate real events. Computers can provide numerical solution of the simulations to a degree of precision that may be limited by the available resources.

Nowadays, computer modelling plays a key role in the developments in the scientific field. Computer modelling is a powerful tool when investigating the relationship between experimental results and theory to support the findings. Models can be tested on the computer and improved as a consequence of modelling results compared with real data in an iterative improvement process. The requirements needed to compare with both theoretical predictions and experimental results can readily be made in computer simulations because of the ease with which inputs can be changed in the computer code.

Development in materials science and industry has been clearly enhanced by the use of computer modelling. Computers provide a 'virtual laboratory' where the response of the material can be
predicted under conditions that are expensive, dangerous, difficult or impractical to produce in the laboratory. One example is the simulation of the materials behaviour for the design of nuclear fusion reactors. Both material properties in service and initial processing conditions can be simulated, allowing for optimisation of manufacturing and correct materials selection at a first attempt without the need for lengthy and expensive experimental trials.

Modelling of materials and industrial processes is not an easy task due to their complexity. A good model of a material has to capture the response of the material in several situations. This model has to take into account that the performance of a material can evolve with time and also all the various mechanisms that contribute simultaneously and synergistically in typical materials problems. Models can be classified in two broad categories empirical and physical. Empirical models use approximations to fit experimental data. Therefore, empirical models cannot contain more knowledge than the data used in its creation. The simplest way to obtain an insight into the process to be described using the data provided is through standard linear regression models. In linear regression, the data can be fitted to a linear form, obtaining as a result a linear dependence between inputs and outputs.

More sophisticated methods like neural networks can be used not only to obtain the linear dependencies but also the non-linear relationships between inputs and outputs that are the most common case in materials behaviour. Neural networks are empirical models that have a proven ability of finding hidden relationships in sets of data. Neural network models have been mainly used in engineering where material problems are so complex that there are no adequate physical models to describe them. There are often large databases concerned with the processes of interest, e.g. welding, which can be presented to a network. Once the network has learnt from the data it is able to predict outputs from a given set of previously unseen inputs of interest.

1.4 Layout of Thesis

Due to the highly involved and complex nature of the modelling technique used in the work, the literature has been divided into two distinct subject areas in order to maintain a clear yet thorough description of the knowledge gained through extensive background research. Firstly Chapter 2 covers the relevant physical metallurgy aspects, and is particularly concerned with the microstructure and effects of the submerged arc welding process. The welding process is
Introduction

detailed, with reference to the consumables, heat effects during welding and any post weld processes, namely mechanical expansion. The various microstructural constituents of line-pipe are then discussed, both in respect of phase transformations that take place during welding and also any post weld re-heating that takes place as a consequence of the second weld pass. Chapter 3 presents an experimental investigation of X100 line-pipe material in which three distinct series of welds, containing different amounts of alloying additions are examined. Optical and transmission electron microscopy (TEM) techniques are used with the aim of determining the inclusion types responsible for the nucleation of fine acicular ferrite in the various steels.

The second literature survey is found in Chapter 4, which discusses the theory and application of neural network techniques in materials science, and in particular to welding processes. The theory and use of the neural network software chosen for this work is discussed in detail. This chapter therefore established an ideal foundation for the modelling work detailed through Chapters 5-8.

Chapter 5 presents the initial modelling work, which was carried out on the relatively simple relationship between parent plate, wire consumable and the weld metal chemistry. From the initial modelling, more complex neural network modelling strategies were developed combining the relatively simple initial models to predict complex multiple outputs for weld metal chemistry. Chapter 5 also includes the prediction of the weld metal acicular ferrite content, from the weld metal chemistry together with heat input characteristics. The amount of acicular ferrite, and a multiple output model for acicular ferrite, primary ferrite and ferrite side-plate are described, and show a high level of confidence in both the predictions made and the influence the model placed on input parameters. The final section of chapter 5 details the use of a binary classification model to predict the occurrence of hydrogen induced cracking (HIC) in a weld. Due to the nature of HIC and the testing procedure required, very few data were available for modelling. Nevertheless, a successful model has been created which produces results to a 95% accuracy level.

The difficult problem of the prediction of the shape of a weld bead is addressed in Chapter 6. Initially only OD welding is considered due to the ease in which the complete bead geometry can be measured. A novel approach to the digitising of the weld bead shape is presented together with the consistent approach used to measure all weld shapes and sizes to avoid any bias in the
neural network in any way. Multiple output models considering the weld bead both as a whole and as distinct regions are discussed, with results showing a high level of confidence compared to previous techniques found in the literature.

Chapter 7 presents successful models that have been developed using the weld characteristics modelled in Chapter 5 and 6, for the prediction of weld metal toughness. Various approaches are discussed, utilising either a chemistry and microstructure input architecture or through the use of more complex inputs involving chemistry, welding process parameters and the weld geometry. A particular success of Chapter 7 is the use made of predictions for acicular ferrite and weld metal chemistry, discussed in Chapter 5, as input values for the modelling of weld metal toughness. This produces excellent results and demonstrates that weld metal toughness can be predicted through the use of process parameters alone.

The application of all of the techniques developed in Chapters 5, 6 and 7 are applied to the more complex problem of the ID weld metal in Chapter 8. The important differences between ID and OD welding are the re-heating that occurs as a consequence of overlaying the OD weld, and the effects of the OD weld preparation during the ID welding process. The key area of this chapter is the prediction of the visible ID weld bead geometry, utilising techniques developed in chapter 6, which when combined with the OD weld bead shape predictions have shown high levels of confidence in the prediction of the complete shape of a submerged arc weld bead.

The conclusions of each area of work are summarised in Chapter 9, and the successful modelling of weld metal geometry, chemistry and mechanical properties though the use of neural network techniques are highlighted. Further work is also considered, and proposals are presented for future adaptation to the manufacturing environment and the possible combination with other modelling approaches.
Chapter 2 – Welding and Metallurgy: Literature

2.1 Introduction

In seam welding of line-pipe the choice of base plate and consumable chemistry, together with welding parameters, to meet the required mechanical property specifications is often based on previous experience. The ability to predict weld metal chemistry is extremely important because the properties of a weld are determined primarily by its chemical composition and cooling rate. Microstructure prediction models, and ultimately mechanical property prediction models, both require weld metal chemistry as their starting point.

Attempts to calculate from first principles the extent of reactions in the weld pool in the case of submerged arc welding have not been very successful to date. Due to the very rapid temperature cycles to very high temperatures during the welding process, the rate controlling steps of the metallurgical reactions in the weld pool are difficult to determine. In addition, reactions are unlikely to reach equilibrium given the short times available during the welding process and the effect of process variables on the extent of reaction is complex. This chapter aims to highlight important process features and complex metallurgical factors that contribute to the various weld characteristics to be modelled in later chapters.

2.2 Welding of line-pipe

Submerged arc welding (SAW) is similar in principle to all other shielded arc-welding processes, involving the formation of an arc between a continuously fed bare wire electrode and work-piece. The process uses a flux to generate protective gases and slag, with inclusion of metal powders to add alloying elements.

2.2.1 Process features

Prior to welding a layer of flux is placed onto the work-piece surface, and the welder moves along the joint line creating an arc beneath the flux. The electric arc formed between the work piece and the electrode creates a plasma consisting of ionised atoms and free electrons with temperatures in the region of 10000°C. The heat generated is carried from the plasma to the work
piece and melting occurs. A weld pool is thus created composed of the material from the work piece and drops of liquid (consumable or filler material) that are produced by the effect of the heat on the electrode. Stirring of the molten pool occurs due to the Lorentz forces caused by the welding current passing through the liquid metal to the parent plate. The complex reactions occurring in the weld pool are indicated in Figure 2.1. As the arc is completely covered by the flux layer, heat loss is extremely low. Thermal efficiency can be as high as 60% (compare this with 25% for MMA – Manual Metal Arc). The arc light is not visible, and the process is spatter free with no need for fume extraction.

Submerged arc welding processes are usually run as fully mechanised or automatic processes. Welding parameters; current, arc voltage, and travel speed all affect bead shape, depth of penetration and chemical composition of the deposited weld metal. As the process is fully submerged, the operator must rely heavily upon the parameter settings the process is illustrated in Figure 2.2.

**Figure 2.1** – Submerged arc welding process dynamics at the weld pool

Fluxes used in submerged arc welding are granular fusible minerals containing oxides of manganese, silicon, titanium, aluminium, calcium, zirconium, magnesium and other compounds such as calcium fluoride. These fluxes are formulated to be compatible with a given electrode wire so that the combination of flux and wire yields the desired mechanical properties through the optimisation of weld metal composition. Submerged arc welding processes are suited for
longitudinal and circumferential butt and fillet welds. Depending on material thickness, either single-pass, two-pass or multi-pass weld procedures can be carried out.

![Diagram of equipment used in the submerged arc welding process](image)

**Figure 2.2** – Outline of the equipment used in the submerged arc welding process

### 2.2.2 Multiple wire welding

The complex phenomena experienced in single wire welding are further increased when more than one welding wire is introduced into the equation, as this complicates the relationship of the thermal cycle to the weld characteristics. During the production of large diameter line-pipe 4-wires are used for inner diameter (ID) welding, and 5-wires for outer diameter (OD) welding. These wires are closely spaced, and therefore molten weld metal is being deposited into an already liquid metal weld pool. A schematic representation of the 3-wire process can be seen in Figure 2.3.
Figure 2.3 - Schematic of 3-wire single pass submerged arc weld metal deposition.

Weld bead shape is an important characteristic for evaluating weld quality; a major factor in weld bead shape is the electrode configuration. Throughout the literature work has been carried out through experimental trials to determine the relationship between electrode set-up for multiwire submerged arc welding and the weld bead shape manufactured\textsuperscript{11-16}. Much is published on the effects of varying voltage, current and welding speed, though little information is available on the subjects of wire interaction; spacing and wire angles on the weld characteristics. Cinderley and Thompson\textsuperscript{16} cover the development of suitable welder set-ups for the 4 and 5 wire welding process using laboratory welders. The report covers the factors determining weld penetration and bead shape, looking specifically at electrode stickout, heat input and electrode spacing using systematic experimental trials. Thompson's earlier work\textsuperscript{15} covers the effect of electrode stickout on heat input, bead size and cooling rate, when considering single wire submerged arc welds. Process variables are also considered in the work by Clarke\textsuperscript{11,12}; his series of papers look at weld process parameters for 4 and 5 wire welder set ups. The work considers the influence of individual wires on the eventual weld bead shape produced, using process inputs, volts, amps, speed, as variable factors.

Bleich et al\textsuperscript{13} consider in detail the effects of changes in electrode configuration for 3 wire submerged arc welding. The effects of changes are assessed in terms of process stability, and measured changes in the weld bead cross sectional area and dimensions. Results are presented showing no obvious effects on arc stability when changing electrode angles, although changes in bead shape and penetration were definitely influenced by electrode angle and spacing set-ups.
The effects of misalignment of the electrodes is covered in the paper by Marsden\textsuperscript{17}, in which parameters are considered which are similar to those used in actual production environments. He compared a fully aligned set-up for 5-wire welding with that of a welder set-up in which the 3\textsuperscript{rd} or 4\textsuperscript{th} wires were misaligned as seen in Figure 2.4. He found that displacing the 3\textsuperscript{rd} and 4\textsuperscript{th} wire resulted in a broader weld with slightly less penetration, and a marginal improvement was seen in fusion line toughness when a more gradual fusion line profile is produced.

In multi-wire welding the lead wire has an applied DC voltage, while the trailing wires carry AC voltages set out of phase with one another. The input of current and voltage to the electrodes is directly related to the heat input to the weld region. Howse and Cochrane\textsuperscript{14} consider constant heat input from single wire multi-pass submerged arc welding. By looking at a series of bead on plate (BOP) and butt welds they were able to consider the influence of weld parameters given a constant heat input. The findings concluded that an increase in current density, either by increasing current for a set wire diameter or by decreasing wire diameter for a set welding current, gave increased weld penetration and weld cross sectional area. Increases in the weld voltage were found to give flatter, wider weld beads decreasing cross sectional area.

![Wires Aligned and Mis-aligned](image)

\textbf{Figure 2.4} – Wire Alignments from the investigation of Marsden adapted from his 1999 paper\textsuperscript{17}
2.2.3 The effects of mechanical expansion of line-pipe

The effects of mechanical expansion are discussed in the report by Thewlis and Dainty\textsuperscript{18} and by McClay et al\textsuperscript{19}, including the strain created in the pipe and weld through both ID and OD welding and the expansion process. An investigation into the strains produced in both pipe body and seam weld in 42 inch pipes was also carried out by Harris\textsuperscript{20}. His report suggests equations to approximate the strain in each manufacturing step and it was shown that compressive strains were found in greater quantities than tensile strains. The O-ing process, described in Chapter 1, was found to produce greater compressive strains on the ID than the tensile counterparts on the OD and the welding process produced compressive strains on both OD and ID beads due to weld shrinkage. Expansion showed varying strains between OD and ID and was also dependent upon wall thickness. Finite element modelling carried out by Wen and Farrugia\textsuperscript{21} has shown that through process residual stress predictions can be made for the different manufacturing stages.

2.3 Composition of a steel weld

Steel is normally produced by casting in the form of an ingot, and then rolling is performed upon the ingot forming plates or other products. Mechanical properties are to some extent affected by rolling temperature and cooling rate from rolling. Mechanical working e.g. rolling or forging, improves the mechanical properties to some degree, but as specifications cover production of material over a range of plate thickness, this means that the range of chemical composition has to be wide enough to achieve the desired mechanical properties. Another factor affecting composition of steel is the presence of small amounts of impurities or trace elements within a weld specification there would be a maximum allowable amount of such elements. The effect is intensified on thicker sections because of concentration of these elements by segregation.

The composition of the weld pool is far more complex to predict as it is made up partly from the filler metal used and partly from parent plate, with possible contribution from the flux. The relative proportions depend upon the type of joint and characteristics of the welding process. Weld metals contain certain elements which, if present in sufficient quantity may segregate to form low melting point films between solidifying grains. Under the action of solidification stresses on these films they may open up into cracks. Most commonly this occurs due to the presence of sulphur, the effect of which further increases with carbon content. Hence, control
of the Mn content is important, due to its ability to control “free” sulphur through precipitation of MnS inclusions.

2.3.1 Consumables

The consumables used in the welding process can be associated with several characteristics of the weld produced and are especially important when considering the weldability of a material. Thewlis\textsuperscript{22} investigates the weldability of X100 line-pipe material, a high strength alloy steel enabling production of line-pipe with thin wall dimensions whilst still operating at higher pressures. The work covers the use of different commercially available consumables to ascertain the optimum parameters for good quality welding of X100 line-pipe. Harold and Thewlis\textsuperscript{23} also look at the weldability of accelerated cooled plate for line-pipe manufacture, looking at X65 and X52 pipe material and consumable alloying on the performance of the weld under sour service conditions. Earlier work by Thewlis\textsuperscript{24} looks at the influence of the parent plate and consumable on the composition, microstructure and toughness of the weld metal. The investigation looks at the conflict between the need for changes in weld and plate composition to meet particular specifications with the changes necessary to develop good weld toughness. Two more papers by Thewlis\textsuperscript{25,26} develop the idea applying the thought process in more detail for longitudinal 3-wire submerged arc welding of line-pipe. Fluxes can be categorised by their basicity index, this is calculated using the equation:

$$B_l = \frac{0.5(FeO + MnO) + CaO + MgO + Na_2O + K_2O + CaF_2}{SiO_2 + 0.5(TiO_2 + ZrO_2 + Al_2O_3)} \text{ wt.}\%$$ \hspace{1cm} 2.1

Tanaka et al\textsuperscript{7} consider the influence of flux composition on the transfer of key elements during submerged arc welding. The investigation looked at the use of fused fluxes with oxides, alloys and simple substances added. The results examining reactions between slag and molten metal, and the usefulness of basicity index and equilibrium equation. The results showed a most interesting phenomenon that TiO$_2$ acted as acid for Ti transfer, but is regarded as basic for the determination of weld oxygen. Davis and Bailey\textsuperscript{27} also consider the influence of flux composition on element transfer in submerged arc welding. The work-investigated data supplied by the ‘Welding Institute’ considering the element transfer from fluxes containing chemical compositions. The report concluded that certain, so called ‘network formers’, allowed better
transfer of certain elements from flux to weld, whilst also considering removal of phosphor (P), carbon (C) and sulphur (S) from the weld, and the necessary composition of fluxes required for this to happen.

2.3.2 Dilution

When two metals are joined together through arc welding processes the final composition of the weld metal consists of a mixture of parent plate and welding wire. Once the parent plate has mixed with the filler wire it becomes diluted; the dilution may be expressed as a percentage as described in the following way:

\[
\text{% Dilution} = \left(\frac{\text{weight of parent metal in weld}}{\text{total weight of weld}}\right) \times 100
\]

Many factors affect dilution. With a single run weld there will be greater dilution than with multi-runs and there is always considerable dilution in any root run. With any first run there is always a greater proportion of the parent plate melted in to the weld than with any consequent runs. This is due to the melting of the weld zone in subsequent runs therefore dilution is lessened. Weaving also increases the amount of dilution; this is used where there is a large gap between plates in comparison to the thickness of the welding wire. This enables for greater penetration of the weld, thus ensuring better fusion of the work-piece. Though the purpose is to deposit a greater amount of filler, hence a greater level of dilution. When dissimilar metals are to be welded, the final weld will suffer dilution from each parent plate. In addition the filler wire must be such that the balance is achieved within the weld metal so as not to compromise mechanical properties.

It must also be noted that any preparation of the work-piece, for example the use of tack welds can have an effect on the final properties of the weld metal. Tack welds are essential in ensuring there is correct gap and line-up of components to be welded. They are usually made with a higher current than normal to ensure good fusion and penetration, they should be strong enough and of sufficient length and spacing to ensure rigidity. This helps to stabilise the work-piece against distortive forces set up during the welding process. The choice of filler and method are of importance to the final result, and must be considered in conjunction with the arc weld parameters so as to optimise weld properties. Composition of the filler rod in comparison with
that of the parent plate is of great importance, since this naturally alters the chemistry and properties of the steel at or near the weld.

If the mass of parent plate is relatively small and cooling is fast, the weld will become strong but brittle, this is due to the formation of martensite. This is particularly the case when carbon content is high. If cooling is controlled, structures of varying forms of ferrite and pearlite are found, giving lower strength and increased toughness, through improved ductility and impact strength. These considerations are of most importance when welding alloy steels since great care is required in the choice of filler rod, to ensure that the weld has the correct properties required. In many cases heat treatment is advised after welding, removing internal stresses and modifying the microstructure, especially with steels such as high tensile and chrome steels.

2.3.3 Movement of material

A self-induced magnetic field is associated with the welding arc; this field interacts with the current producing a force on charge carriers. A local region of high pressure is created in opposition to the electromagnetic force. As the arc is not of equal cross-sectional area throughout a relatively higher region of pressure occurs at the electrode tip causing arc plasma to flow away to areas of lower pressure, the weld pool surface. Much understanding of metal transfer in arc welding comes from gas shielded welding systems. Today through the use of X-ray techniques, it can be shown that metal transfer behaviour is similar to that in gases.

The forces to consider upon the droplet at the electrode tip are:

- Gravity
- Plasma jet action
- Restraining Force ⇒ Surface Tension

At high currents, as the electrode melts a droplet grows in diameter. If the velocity of the plasma jet were to remain constant, the force per unit area exerted upon the droplet would increase with increasing droplet size, until it was sufficient to overcome restraining forces; the plasma jet then detaches this. With a low current, the velocity and hence force per unit area is decreased whilst restraining forces remain constant, thus globule size must increase before detachment can take
place. The detaching force at low currents is a balance between surface tension, droplet size, gravity and plasma jet force, with plasma jet force being the dominating influence at higher currents, resulting in smaller drops. The intensity and duration of any chemical reactions between weld metal and surroundings, is related to droplet sizes and so called lifetimes. The dimensions of droplets, and time for transfer can be related to:

**Welding conditions**
- Electrode polarity
- Type of current
- Formation or lack of formation of plasma jet

**Characteristics of the welding wire and surrounding environment**
- Composition
- Density and viscosity of environment
- Interface tension

Basic transport processes in the weld pool are diffusion, natural convection known as buoyancy, and forced convection driven by Lorentz forces occurring from the passing of current through the molten pool and the gouging of the welder travel. These forces all cause motion and circulation of constituents, the rate of mixing and circulation of reactive constituents diluted into the weld pool from the parent plate may therefore be related to the source of motion.

2.4 **Absorbed and alloyed elements**

It can be shown that when an arc is struck and weld pool formation occurs, ions from the shielding medium are driven across the welding arc by the pumping action of the arc plasma. Work on flux shielded arc systems show that reactions may take place at:

i. The surface of the droplet at the electrode tip
ii. The surface of the droplet during flight
iii. At the arc root
iv. Away from the arc root at the weld pool surface
Very high temperatures in the arc plasma favour reaction in the droplet at the electrode tip and during droplet flight, though as previously mentioned droplet sizes and lifetimes limit reactions.

2.4.1 Element transfer

Pick-up is the term applied to the absorption or transfer of elements from parent-plate or non-consumable electrode into the weld metal, and is closely associated with dilution. This can lead to anomalies in the structure and properties of the weld and must therefore be kept to a minimum. Slag/metal reactions also play a major role in the determination of weld metal compositions during submerged-arc welding. Therefore much attention must be placed on element transfer from flux to weld metal.

2.4.2 Inclusion formation and distribution

Electro-magnetically induced motion in the liquid weld metal acts in sweeping reaction products from the weld surface in to the body of the weld. This causes further reactions to occur between reactants entrained within the flow patterns, the degree of reaction is dependent upon the reactivity of the product and the severity of the mixing motion.

Inclusion formation and distribution in the liquid metal weld pool is closely related to the influence of weld pool motion, determining dominantly the rate of reactions and degeneration of the reactants.

2.4.3 Oxygen

Oxygen absorption affects the weld in three ways; through the precipitation of non-metallic inclusions, oxidation of alloying elements, and CO porosity. The iron oxide may be absorbed in to the weld from the steel of the electrode or welding rod or from arc atmosphere. If iron oxide is formed, a reaction may occur with carbon in the steel forming carbon monoxide; this will result in the appearance of blowholes or porosity. If iron oxide becomes present in any quantity, oxidation of the weld will occur producing a great increase in grain size, even normalising will the not produce a fine grain. Oxygen absorption therefore has a bad effect upon weld properties, increasing brittleness, reducing tensile strength, and decreasing resistance to corrosion.
Deoxidising materials may be added to remove iron oxide; silica in sufficient amounts will remove it to form an iron silicate slag.

It is important when considering the mechanical properties of a weld, to consider oxygen composition, especially with regard to toughness. To improve toughness in submerged-arc welds the oxygen contents of the deposit must be minimised.

TiO$_2$ was found to be more effective in reducing oxygen than Al$_2$O$_3$ in spite of their classification as amphoteric. It was also observed that basic constituents such as CaO and MgO gave lower weld oxygen contents than amphoteric constituents. Thus considerable emphasis is placed on the concept of basicity of submerged-arc fluxes as a means of producing low oxygen content weld metals.

Oxygen content or basicity can be determined to some extent by the use of the $B_L$ value (Mori index) except where fluxes contain much TiO$_2$, regardless of differing weld conditions or Si and Mn content of plate and wire. $B_L$ is found by using equation 2.3.

$$B_L = 6.05N_{CaO}+4.8N_{MnO}+4.0N_{MgO}+3.4N_{FeO}-6.31N_{SiO2}-4.97N_{TiO2}-0.2N_{Al2O3}$$ \hspace{1cm} (2.3)

where $N_i$ is representative of the mole %

Increase of basicity ($B_L$) reduces oxygen content. Since TiO$_2$ is classified as acidic, therefore an increase of TiO$_2$ decreases basicity index $B_L$. Though large additions of TiO$_2$ to the flux reduced weld oxygen content, therefore the results cannot be explained solely by the basicity concept. It is therefore reported that the oxygen potential during welding should be considered as the important factor in the determination of the transfer of oxygen to the weld metal during submerged-arc welding, see Tanaka et al$^7$.

Oxygen potential during steel making is generally considered as the partition of oxygen between metal and slag, and is related to the ferrous oxide of the slag. The oxygen partition is determined using equation 2.5:

$$[\text{Fe}] + [\text{O}] = \text{FeO}\hspace{1cm} (2.4)$$
The percentage of nitrogen absorbed in weld metal can vary considerably, with greater absorption occurring during arc welding processes. The amount absorbed can be linked to the partial pressure of nitrogen in the arc atmosphere. Nitrogen is found in weld metals trapped in blowholes (though the nitrogen itself does not form these blow-holes), and as iron nitride crystals (Fe₄N) also known as nitride needles. Nitrogen may also appear in solution in the iron, and this must be heated to between 800-900°C for it to form into iron nitride needles. Nitrogen tends to decrease the ductility of the metal, but increase the tensile strength.

High levels of nitrogen in the weld metal have been shown to have a detrimental effect on the weld metal toughness; this can clearly be seen throughout the literature. Free nitrogen content of the weld metal should increase the matrix strength and adversely influence the impact transition temperature. Aluminium has differing levels of influence on the toughness of the weld metal, though this has a critical relationship to the amounts contained. Any level of calcium can be seen to have a detrimental effect upon the toughness of the weld metal.

An increase in nitrogen in weld metal raises the level of free nitrogen, thus removing the soluble boron as boron nitride, whilst further nitrogen combines with titanium as titanium nitride particles. Changes in primary ferrite content occur depending upon whether the increase in nitrogen causes an increase in free or combined nitrogen. From the literature it is seen that prior austenite grain size becomes finer with increase of the nitrogen content of the weld deposit. Though evidence is also present to suggest that inclusions present may pin the weld metal prior austenite grain boundaries. Increase in the nitrogen content of the weld metal, by increasing the
volume fraction of boron nitride particles should therefore lead to an increase in grain boundary pinning and a refinement of the prior austenite grain as observed.

2.4.5 Hydrogen

Hydrogen is absorbed into mild steel weld metal during arc welding from flux materials. The hydrogen is present in many flux coatings and powders, and in their moisture content. Hydrogen begins to diffuse out of the weld metal immediately after the welding process and continues over a long period. Hydrogen results in the reduction in the tensile strength of the weld metal.

Hydrogen embrittlement can be considered a serious problem with welding, and is closely associated with lamellar tearing. Hydrogen is associated with two forms of damage within a weld, the first occurs at high temperature and affects carbon and low-alloy steels. This occurs due to chemical reactions taking place between hydrogen and carbides; this causes permanent damage by decarburisation and cracking. The second form of damage occurs in the temperature range; 100°C to 200°C. This type of embrittlement is due to the physical interactions between hydrogen and the crystal lattice; this is reversible in that after removal of the gas the ductility of the steel reverts to normal.

2.4.6 Carbon

Introduction of additional carbon into the weld metal results in either oxidation into carbon monoxide during the melting operation or reaction with the weld metal and production of a porous deposit. Arc welding processes produce high cooling rates, and thus the material can be expected to be brittle therefore introduction of carbon must be lower for arc welded processes.

The effect on the weld metal of carbon contained in the parent metal is also of high importance, especially when welding medium or high carbon steels. The carbon may diffuse from the parent plate, due to the relatively high carbon content, into the weld metal and form near the line of fusion. Bands of high carbon content form, being sufficient to cause local hardness and brittleness if cooled rapidly.
The rate at which ferrite grows, increases sharply as carbon concentration of the steel approaches its solubility in ferrite. The reason for this is that there is no need for carbon to diffuse ahead of the γ/α interface, since it can all be accommodated in the ferrite. Changes in the mechanical properties reflect this, the strength of low-carbon steels being sensitive to the carbon concentration. Carbon in effect controls the kinetics of transformation.

Hardenability of the steel, when considered from a welding point of view is usually expressed as a carbon equivalent (CE). Each element is scaled relative to its ability to retard the γ/α transformation. Steels with a CE in excess of about 0.4wt.% cannot easily be welded due to their tendency to form martensite. The CE can be expressed using the following expression:

\[
CE = C\% + \frac{Mn\%}{6} + \frac{(Cr\% + Mo\% + V\%)}{5} + \frac{(Ni\% + Cu\%)}{15}
\]

2.4.7 Other important alloying elements

Weld metal composition is determined from flux, wire, and plate composition. A convenient way of studying the effect of flux constituents is to compare the analysed composition with that expected. Expected composition is derived from wire and plate compositions and dilution as follows:

\[
\text{Expected comp.} = (\text{Dilution}/100) \times \text{plate comp.} + (1-(\text{dilution}/100)) \times \text{wire comp.}
\]

Dilution is expressed as a %.

\[\Delta M = \text{Analysed comp.} - \text{Expected comp.}\]

\[\Delta M\] is used to rationalise the changes of elements as a function of flux composition. If \(\Delta M\) is greater zero, the element M is considered to transfer from slag to weld metal. Addition of alloys or simple substances led \(\Delta Si\) and \(\Delta Mn\) to the positive direction; in particular the affects of adding Ti, Al, Mg and Ca. Oxides such as TiO\(_2\), Al\(_2\)O\(_3\), MgO and CaO are stable at high temperature. MnO and SiO\(_2\) are deprived of oxygen by Ti, Al, Mg and Ca additions during submerged-arc welding, resulting in Si and Mn transfer from slag to metal.
Ti can be efficiently transferred with increasing basicity index. Moreover, Al and Mg additions to TiO₂ containing fluxes helped transfer of Ti more efficiently from flux to weld metal. This is because oxides such as Al₂O₃ and MgO are more stable than TiO₂ from the subject of formation energy of oxide, so TiO₂ in molten slag is deprived of oxygen by Al and Mg additions, resulting in transfer of Ti to weld metal. Boron (B) acts differently to Ti, with basicity of the flux having little influence on transfer to weld metal. Tanaka et al found that addition of 0.5 wt.% B₂O₃ resulted in weld metal with 50 ppm B content. Agreeing with findings of earlier research of Tsunetomi et al.

2.5 The effect of welding on the microstructure of steel

During the welding process, high temperatures are experienced by the steel work-piece, with the thermal cycle taking only a relatively short period of time to occur. This has an effect upon the resultant microstructure formed in the final as-deposited weld metal. Along with the influence of the thermal cycle, the alloying additions play an important role in the final microstructure, and can be used to closely control the quantities of a given phase. This section discusses the types of microstructure experienced in the X65 and X100 weld metal examined in this thesis.

2.5.1 Weld metal thermal cycle, melting and reactions

The temperature cycle for a single wire arc weld, shown in Figure 2.5, is relative to the input amps, volts, welding speed and cooling rate. This thermal cycle is further complicated when multiple wire set-ups are used. Heat removed is determined by the apparent heat sink relative to the size of the parent plate and weld bead. This relationship, coupled to the type of weld preparation, governs the amount of dilution of parent plate occurring.

A series of chemical reactions between liquid metal and shielding element (gas, flux) take place during arc welding processes. The factors affecting the weld metal properties in arc welding are covered by Thewlis looking at the outcome of the interactive influence of the weld parameters and consumables. Previously there have been many attempts to calculate the metallurgical reactions within the submerged-arc process, theories being mainly based upon metallurgical thermo-chemistry. There are two main reasons for the failure of many approaches to modelling
the welding process and characteristics of resulting welds, highlighted in the work of Thier and Killing\textsuperscript{29}.

During the welding process the metal takes an unknown temperature cycle from room temperature to about 3000K and back to room temperature, this cycle shown in Figure 2.6. In addition to this velocity and velocity controlling steps of metallurgical reactions are unknown. Reaction time during the welding process is so short, that thermodynamic equilibrium cannot be expected to be reached. In addition the extent of metallurgical reactions are dependent upon welding parameters, such as heat input, alloying elements used, preparation of parent metal, weld speed and number of passes or wires in weld process.

Heat input is influential in many characteristics of the weld, determining microstructural and physical attributes. Lee et al\textsuperscript{30} consider the process inputs related to the occurrence of bay area in submerged arc welds. The observations state that the formation of bay area in weld beads is influenced by the heat distribution from the arc, being determined by the welding conditions.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.5}
\caption{Temperature Cycle of Metal During Arc Welding Process adapted from Thier\textsuperscript{31}}
\end{figure}

The welding process involves a source of intense heat, the main purpose of which is to cause melting; the cooling that follows leads to the formation of an integral joint. Much of this heat is diffused into the atmosphere and surrounding material and as a consequence the surrounding
material experiences heating and cooling cycles, the magnitude of which is dependent upon the distance from the fusion line; peak temperature and fusion rate decrease with distance away from the fusion boundary. The cooling rate is less sensitive to the distance from the heat source; this cooling is usually represented as the time taken to cool from 800-500°C, $\Delta t_{s.5}$. In many weldable steels this defines the temperature range at which austenite decomposes by solid-state transformation. The thermal cycle can therefore be characterised by two parameters, the peak temperature $T_P$, and time period $\Delta t_{s.5}$, both increasing with heat input.

A typical cross-section from the molten pool to the cold section of the parent plate at a particular time interval might reveal the following, also shown in Figure 2.6:

a. The molten pool with parent plate and weld metal mixed at temperatures above the melting point, 1500 °C.

b. A region of BCC delta iron and austenite (FCC gamma iron) mixed - Above 1400 °C.

c. A region of austenite above the upper critical temperature - 900°C.

d. A region of austenite and ferrite (BCC alpha iron), where ferrite is being precipitated between upper and lower critical temperatures) - 720-900 °C.

e. The parent plate of ferrite and pearlite - Below 720 °C.

Figure 2.6 – Types of iron present following welding steel plate adapted from Davies^32
The microstructure obtained as the weld cools from the liquid phase to ambient temperature is known as the as-deposited microstructure. This consists of three major components; allotriomorphic ferrite, Widmanstätten ferrite and acicular ferrite. Martensite, retained austenite or degenerate pearlitic may also be present in relatively small quantities, and are known as micro- phases. Bainite, consisting of sheaves of parallel platelets, is not usually found in a well-designed welding alloy. This is because acicular ferrite is induced to nucleate heterogeneously on non-metallic inclusions.

With multi-run welds a complicated structure is formed. The regions of as-deposited microstructure are reheated to temperatures high enough to cause reformation of austenite, which during cooling causes partial transformation into other structures. The deposit of subsequent runs may simply temper other regions. This new microstructure is known as the reheated or secondary structure. The change in the microstructure is dependent upon:

- The process used and process parameters (e.g. heat input)
- Type and composition of filler rod and flux addition
- Environment conditions under which the weld is made. (Presence of nitrogen, oxygen etc.)
- Composition of the parent plate.

The change in structure of the weld metal is highly dependent on the amount of carbon present and other alloying elements and the rate at which the weld is cooled. In arc welding the first run of weld metal onto the cold plate is virtually chill cast; the metal on top of the weld area freezes quickly as the heat is removed from it and small chill crystals grow away from the sides towards hotter regions of the weld metal. Due to the high temperatures involved in arc welding processes, the crystals have time to grow. Growth of grains is therefore faster than the tendency to form new dendrites so that columnar crystals are formed. A heat-affected zone (HAZ) is present on each side of the weld, in which the temperature has been raised above the recrystallisation temperature, and therefore grain growth has occurred.
Beyond the HAZ the plate is unaffected. Further structural changes will occur when a second run is placed over the first, these are:

- A refined area in the first run where the recrystallisation temperature is exceeded and the columnar crystals of the first run are reformed as small equi-axed crystals.
- A region between this and the parent plate where grain growth has taken place because the temperature has been well above recrystallisation temperature.
- The second run will form columnar crystals on its lower surface layers because of the quick cooling when in contact with the atmosphere.

There are several temperatures or critical points in the diagram, Figure 2.7, which are important, both from the fundamental and practical points of view. Firstly there is the $A_1$ temperature at which the eutectoid reaction occurs at 723°C. Secondly there is the $A_3$ temperature, when the $\alpha$-iron transforms to $\gamma$-iron. For pure iron the corresponding temperature is 910°C, though the transformation temperature is progressively lowered with increasing carbon content. The third point, the $A_4$ temperature at which $\gamma$-iron transforms to $\delta$-iron, at a temperature of 1390°C for pure iron, increases with increased carbon content. The fourth point, the $A_2$ temperature or better known as the Curie point, is when iron changes from the ferro- to the paramagnetic condition. The temperature corresponding to this is 769°C for pure iron, with no change in crystal structure being involved.
2.5.2 Fusion Zone

The weld deposits begin solidification with the epitaxial growth of columnar delta-ferrite (δ), growing from the hot grain-structure of the parent plate at the fusion surface. Grains are anisotropic, growing along the direction of heat flow. Grains with their direction of growth parallel to the heat flow grow fastest and hence hamper the development of those oriented differently. During the solid-state transformation of δ-ferrite to austenite, the austenite nucleates at the δ-δ grain boundaries and develops as a columnar austenite grain structure, with falling temperature. Details of shape and size of the austenite grains is of importance in the evolution of the final microstructure.
The effect of the austenite grain size is two fold:

1) The number density of austenite grain boundary nucleation sites changes inversely with the grain size. Coarse-grained weld deposits have a higher hardenability.

2) More subtly, the effect of columnar shape of the austenite grains, similar in shape to a hexagonal prism. Grains are typically 100µm by 5000µm, being quite unlike an equi-axed grain structure, and due to the fewer grain boundary interactions involved, hardenability can be larger than that of wrought iron.

Solidification does not happen under equilibrium conditions in a weld. Therefore the microstructure is classed as inhomogeneous, as solidification-induced chemical segregation arises due to uncontrolled changes in the welding process. The amplification of these variations becomes larger as alloy content of the steel increases. Fluxes employed in the protection of the hot weld metal can lead to an increase in oxide inclusion in the weld. These oxide particles becoming trapped in the fusion zone during the solidification process. These inclusions serve as heterogeneous nucleation sites and are of considerable importance to the evolution of the microstructure.

2.5.3 Transformation Products

The point and conditions at which transformation structures are formed in weld metals are difficult to define, as there is a certain degree of overlap in conditions whereby a particular transformation begins and the former ends. There is general agreement throughout the literature that the different transformation structures in weld metals in order of decreasing temperature are as follows:

i. Grain boundary primary ferrite
ii. Widdmannstätten ferrite, or ferrite side-plate
iii. Acicular ferrite – also considered as intragranularly nucleated bainite
iv. Upper bainite

The IIW have developed a scheme for the identification of ferritic weld metal microstructural constituents. This scheme aims to achieve international agreement on terminology for the
description of constituents. The scheme was initially proposed in IIW Doc. IXJ-29-80; this was later revised in 1985, and again in 1988 in the "guide to the light microscope examination of ferritic steel weld metals". Definitions of the microstructure constituents found in the line-pipe material, investigated in this thesis, are defined using the IIW scheme as follows.

**Primary ferrite - PF**

This may occur in two forms, which are considered as separate constituents.

- Grain boundary ferrite (veins of polygonal grains) associated with prior austenite grain boundaries. An example of primary ferrite found on a prior austenite grain boundary surrounded by a matrix containing mainly acicular ferrite is shown in Figure 2.8, taken from X100 line pipe steel.

- Intragranular polygonal ferrite Ferrite grains, usually polygonal, found within prior austenite grains and which are larger than about three times the average width of surrounding AF or FS laths are referred to as intragranular polygonal ferrite. Note the term lath is used in the description of the individual ferrite forms, which go to make up a region of AF, acicular ferrite, or FS, ferrite with second phase.

![Grain boundary primary ferrite, PF, on a prior austenite grain boundary surrounded by acicular ferrite, AF, matrix, from X100 line-pipe steel.](image)

**Figure 2.8** - Grain boundary primary ferrite, PF, on a prior austenite grain boundary surrounded by acicular ferrite, AF, matrix, from X100 line-pipe steel.
Acicular ferrite – AF
Small non-aligned ferrite grains found within prior austenite grains, defined as a highly chaotic structure. A region of AF often includes isolated laths of high aspect ratio. Examples of acicular ferrite can be found in Figure 2.8 and Figure 2.9(a).

Ferrite sideplate – FS
This occurs in two forms, considered as separate constituents, examples of both can be seen in Figures 2.9.

Aligned ferrite side-plate [FS(A)] is recognised where two or more long parallel laths of ferrite are seen. Where there are only two laths, these should only be classed as FS if their aspect ratio is greater than 4:1, otherwise they are classed as AF or PF. Other distinctions can be made in identifying these phases as side plates, upper bainite or lower bainite.

Non-aligned ferrite side-plate – [FS(NA)] defined due to growth out of the plane of examination, the ferrite is found to be completely surrounding either (i) microphases that are approximately equi-axed and randomly distributed and (ii) isolated laths of acicular ferrite.

Figure 2.9 – (a) example of non-aligned ferrite side-plate, FS(NA), and acicular ferrite, AF, taken from X100 line-pipe material (b) example of aligned ferrite side-plate, FS(A), taken from X100 line-pipe material at 100x magnification
Martensite has also been recorded in a few examples of welding, though not in any consistent numbers. Martensite is recognisable as very fine microstructure, being sub-categorised as either lath or twinned martensite, though this is not usually possible with optical methods. Colonies of martensite found within prior austenite grains form to be larger than adjacent ferrite laths, whereas smaller colonies should be treated as microphases.

2.5.4 $\delta \rightarrow \gamma$ Transformation

Upon cooling, weld metal of composition less than 0.1wt.% C must pass through the dual phase $\delta + \gamma$ region before entering the single-phase $\gamma$ region. Throughout the literature there is little to be found about the mechanism of this weld metal transformation, though there is strong belief that the transformation occurs by the nucleation of austenite at $\delta$ grain boundaries or solute rich sub-boundaries\(^{34}\). It must be noted that the cooling rate through the $\delta + \gamma$ region is very fast. On cooling the weld metal into the austenite temperature range, austenite grain boundary migration may occur, though the major school of belief is that inclusions pin the migrating boundaries. Inclusion size and distribution can therefore be related to the extent of grain boundary pinning that takes place, the greater this pinning effect, the finer the austenite grain size.

2.5.5 $\gamma \rightarrow \alpha$ Transformation

Allotriomorphic ferrite ($\alpha$) is the first phase to form on cooling the austenite grains below the $\mathrm{Ae}_3$ temperature ($\gamma \rightarrow \alpha$ transformation start temperature), nucleating at the columnar austenite grain boundaries, which are relatively easy diffusion paths and therefore become decorated with thin, continuous layers of ferrite. These layers thicken at a rate controlled by the diffusion of carbon in the austenite ahead of the transformation interface. Assuming isothermal conditions, the ferrite thickness $S$ changes according to the equation defined by Honeycombe and Bhadeshia\(^{35}\).

\[ S = \alpha_1 t^{1/2} \]

\( \alpha_1 \) - Parabolic rate constant \hspace{1cm} t - Time
The parabolic rate constant ($\alpha_1$) is dependent upon the equilibrium compositions of austenite and ferrite, and the diffusivity of carbon in austenite phase. The introduction of manganese, known for stabilising effect on austenite, is associated with low $\alpha$ values, for example. It must be remembered that processes involved with welding are not isothermal, however as nucleation is not rate limiting, the fraction of allotriomorphic ferrite obtained correlates directly with the parabolic rate constant.

Alloying elements such as molybdenum and boron are especially important in controlling transformation temperature and obtaining specific weld metal microstructure, during the cooling of weld metal through the austenite temperature range. From the literature it can be seen that boron influences the $\gamma \rightarrow \alpha$ transformation by diffusing to the grain boundaries and retarding the transformation kinetics of austenite$^{36}$. Suppression of the $\gamma \rightarrow \alpha$ transformation at the austenite grain boundaries, results in the nucleation and growth of ferrite in the intragranular regions.

Considering the $\gamma \rightarrow \alpha$ transformation, given a particular weld metal cooling rate, the temperature at which austenite transforms and nucleation occurs in the intragranular regions may be related to the following, as stated in the 1985 paper by Thewlis$^2$:

i. Weld metal alloy content (boron, molybdenum).
ii. Austenite grain size (grain boundary pinning by inclusions).
iii. The number of austenite grain boundary triple points.
iv. The surface area of high angle austenite grain boundaries.
v. Inclusion/particle size, number, spacing and location (weld metal oxygen content).
vi. Inclusion/particle surface chemistry/strain effects in the surrounding matrix.

Increasing the number density of inclusion nucleation sites relative to austenite nucleation sites, favours the formation of acicular ferrite. Therefore refinement of the austenite grain size or reduction of oxide content below a limiting value leads to the decrease in acicular ferrite content.
2.5.6 Acicular Ferrite Formation

Nucleation of acicular ferrite (AF) begins at the austenite grain boundaries; once initiated the process is continuous at grain boundaries and in intragranular regions as the transformation proceeds. Acicular ferrite nucleates at the austenite grain boundary at around 700°C, dominantly at triple points and points associated with inclusions, growing in either elongated or granular form. Upon further cooling nucleation of AF on larger inclusions is seen to start at around 600°C within the intragranular regions.

Through the cooling range 600-400°C, we see further growth of the AF laths aligned along the prior austenite grain boundaries. Within the intergranular regions, growth of AF may continue from larger inclusions whilst nucleation is observed to start upon the smaller inclusions/particles. More carbon can be seen to diffuse into the remaining austenite region forming pools of carbon-rich austenite, trapped amongst the growing AF grains these are either retained as austenite or are transformed to ferrite plus carbide or martensite.

Thus it can be seen that the formation of acicular ferrite in weld metal is dependent upon:

- Retardation of the nucleation of ferrite at the austenite grain boundaries.
- Retardation of the growth rate of ferrite nucleated at the austenite grain boundaries.
- Encouragement of a high nucleation rate of acicular ferrite on inclusions and dislocation substructures in the intragranular regions.
- Retardation of the growth rate of ferrite in the intragranular regions.

2.5.7 HAZ (Heat Affected Zone)

Local application of heat energy is applied in order to bring the material to a temperature, at which it will fuse, for steels this is between 1400-1500°C. This energy is dissipated into the surrounding atmosphere and into the parent plate material. During welding a temperature gradient is set up in the material ranging from the fusion temperature in the weld pool down to the initial plate temperature some distance from the weld, as represented in Figure 2.7. The material adjacent to the weld, even though it does not melt, undergoes a severe thermal cycle as a
result of welding and because of this micro-structural changes may occur in those regions, known as the heat affected zone (HAZ). The extent of changes that take place, are dependent upon the composition of plate and the rate of heating/cooling in the thermal cycle.

Using a time-temperature-transformation plot (TTT), as seen in Figure 2.10, the subsequent phases formed during HAZ heating can be determined. For typical heating rates encountered in the region adjacent to the fusion boundary, the formation of austenite should be completed when the temperature has exceeded $A_{e3}$ temperature, the fully austenitic temperature, by about 100°C. Since peak temperature ($T_p$) in this zone is much higher than $A_{e3}$, the austenite grains coarsen rapidly as $T_p$ is approached. Once coarsening begins it proceeds very rapidly because the effect of temperature increases exponentially during heating, due to diffusion. The coarsening of the austenitic structure is therefore determined by the applied re-heat temperature and rate of cooling, determining any prolonged thermal effects.

![TTT diagram](image)

**Figure 2.10** – A TTT diagram typical for steels adapted from Svensson

The importance of the coarse-grained austenite zone is in the mechanical properties that develop as the austenite transforms during the cooling part of the thermal cycle. Coarse grain structure
leads to an increase in hardenability, with untempered martensite and other hard phases forming during cooling. Welding introduces atomic hydrogen into the weld metal, which is able to diffuse rapidly into the heat-affected zone. Hard microstructures are particularly susceptible to embrittlement by hydrogen; the fracture occurring shortly after the weld has cooled to room temperature. This phenomenon is known as ‘cold cracking’ and is the reason why the carbon equivalent (CE) must be kept low enough to prevent the hardness in the coarse grained region from becoming unacceptably large.

In order to optimise the re-heated structure it is desirable to obtain a fine-grained austenitic region, typically recognised by austenite grains 20-40μm in size. The grain structure and hardenability are therefore not very different from those associated with control-rolling operations during the manufacture of the steel. The fine austenite grains thus transform into more desirable ferritic phases, with lower hardness values and higher toughness.

At a distance sufficiently large enough from the fusion boundary, the peak temperature is such that the steel cannot transform completely to austenite, known as partially austenitic regions. Though small amounts of austenite are formed they largely have a higher carbon concentration, this is due to the solubility of carbon in austenite in equilibrium with ferrite, increasing with decrease in temperature. The transformation behaviour that follows of the enriched austenite is quite different, since it has a higher hardenability; creating local brittle zones.

If the rate of cooling is sufficiently large, then carbon-enriched austenite will transform partially into hard martensite, the remaining austenite being transformed to ambient temperature. The term used to identify these regions of hard martensite is ‘local brittle zones’, usually situated in the much softer surroundings of tempered ferrite. This does not lead to a general decrease in toughness, but an increase in scatter associated with toughness tests, due to the sample for testing only accounting for the local brittle zone. When cooling rate in the region is not sufficiently high enough to induce martensitic transformation, carbon-enriched austenite decomposes into a mixture of coarse cementite and ferrite. Cementite particles constituting local brittle zones, increasing variability of mechanical properties.
2.6 Chapter Summary

The aim of this chapter has been to highlight areas within the literature important to understanding the fundamentals of the characteristics of welding, covering welding techniques and metallurgical aspects. The literature covered highlights the complex relationships between welding parameters and the as deposited weld characteristics. These fundamental principles are important as a background for evaluating the modelling processes covered later in this thesis.

Throughout the literature it is clear that many attempts have been made to calculate from first principles the extent of reactions in the weld pool in the case of submerged arc welding, and have not been very successful to date. Due to the very rapid temperature cycles to very high temperatures during the welding process, the rate and the rate controlling steps of the metallurgical reactions in the weld pool are difficult to determine. In addition, reactions are unlikely to reach equilibrium given the short times available during the welding process and the effect of process variables on the extent of reaction is complex.

Alloying elements play a vital role in producing a high quality weld, being used as reaction initiators and nucleation sites, allowing control over the eventual microstructure formed. The influence of various alloying elements used in the welding of steel line-pipe, have been discussed highlighting the improved properties gained, or reduction in weld quality caused by so-called impurities inevitably present in the plate and consumables. Consideration of such detailed chemical analysis is important when evaluating the modelling in later chapters.

By gaining an understanding of the metallurgical aspects surrounding the modelling of line-pipe seam welds, the arguments used in evaluating the neural network models can be underpinned by knowledge of the controlling physical metallurgy principles together with neural network modelling literature discussed in chapter 4.
Chapter 3 - Microscopy techniques applied to X100 line pipe material: Analysis

3.1 Introduction

With any type of modelling it is important to gain an understanding of the background surrounding the subject being modelled. Therefore to gain knowledge of the metallurgy of line-pipe welds optical and electron microscope techniques were used to investigate X100 weld material. This chapter will cover the theory behind the techniques to be used in evaluation of these welds, and discuss the findings of the work.

Three sets of submerged-arc welds were manufactured at the Corus Technology Centre in Rotherham, with the aim of obtaining a series of welds with progressively increasing levels of alloying. This was obtained by a combination of different plate and consumable chemistries. Representative samples from each series were selected for investigation using both optical and electron microscopy techniques. The various techniques allowed a more detailed examination of the welds, which took into account the contribution of the inclusions and matrix to the properties of the weld metal. The optical microscopy work carried out presented a picture of the type of microstructure present within the weld metal. This showed that with increasing alloy content of titanium, the nucleation and growth of acicular ferrite was seen to increase.

By undertaking these investigative exercises a knowledge of the metallurgy involved with welding of line-pipe steels could be gained through a hands on approach. The hands on approach enabling explanation of the findings from modelling of the various weld metal characteristics with a sound metallurgical knowledge to both support and explain the findings of the work in this thesis. Examination of the X100 weld metal using electron microscopy techniques was also aimed at carrying on from research carried out at the Corus Technology Centre\textsuperscript{22}; where the characterisation of the weld metal was considered as a whole. The electron microscopy techniques enabled deeper exploration of the weld metal, involving examination of the chemical make-up of the inclusions and the orientation of nucleating ferrite microstructures. The analysis of all welds led to the finding that regardless of the levels of alloying elements, the structure of the matrix was found to be BCC throughout as expected. Inclusions were found to
have either a FCC or a BCC structure. The analysis of inclusions using energy dispersive x-ray (EDX) analysis in many cases showed that surface chemistry differed from the chemistry at the centre. Results revealed a higher level of titanium in the centre of inclusions than on the outer edge of the inclusion, in most cases, when compared with levels of aluminium, silicon and manganese. Also with decreased weld titanium content the size and volume fraction of ferrite laths increased while the acicular ferrite content decreased.

3.2 Microscopy analysis techniques

3.2.1 Light microscopy

Visible light is focused through a specimen by a condenser lens, then is passed through two more lenses placed at both ends of a light-tight tube. The latter two lenses each magnify the image. Limitations to what can be seen in bright field microscopy are not so much related to magnification as they are to resolution, illumination, and contrast. Resolution can be improved using oil immersion lenses, and lighting and contrast can be dramatically improved using modifications such as dark field, phase contrast, and differential interference contrast.

3.2.2 Transmission electron microscopy (TEM)

In transmission electron microscopy (TEM), a beam of highly focused electrons is directed toward a thinned sample (<200 nm). These highly energetic incident electrons interact with the atoms in the sample producing characteristic radiation and particles providing information for materials characterisation. Information is obtained from both deflected and non-deflected transmitted electrons back scattered and secondary electrons, and emitted photons.

3.2.3 Application of the TEM

As previously mentioned the electron beam passes through the sample, revealing the interior of the specimen; the structure size, shape, and distribution of phases can be quantified using this technique. Through the use of energy dispersive x-ray techniques the composition and distribution of the elements can also be determined. The wavelength of electrons is much smaller than that of light; the optimal resolution attainable for TEM images is therefore many orders of
Microscopy techniques applied to X100 line pipe material: Analysis

magnitude better than that from a light microscope. Thus, TEM can reveal the finest details of internal structure - in some cases as small as individual atoms. Images obtained from a TEM are two-dimensional sections of the material under study, but applications that require three-dimensional reconstruction can be accommodated by these techniques.

The energy of the electrons in the TEM determine the relative degree of penetration of electrons in a specific sample, or alternatively, influence the thickness of material from which useful information may be obtained. Thus a 400 kV TEM not only provides high resolution but also allows for the observation of relatively thick samples (e.g. less than 0.2 micrometers) when compared with the more conventional 100 kV or 200 kV instruments.

3.2.4 TEM imaging and analysis techniques

Bright Field imaging - This imaging mode takes advantage of mass contrast diffraction to image the internal microstructure of materials; commonly used in the imaging of grain and defect structures, for example dislocations and voids. Second phases such as precipitates and inclusions are also easily observed by this technique, with features in the range of several hundred μm be easily observed.

Dark Field Imaging - A similar technique to that of bright field, making use of specific so-called Bragg diffracted electrons to image the region from which they originated. This allows linking of diffraction information with specific regions or phases in the sample.

Electron Diffraction - It is possible to view and record the electron diffraction pattern from selected areas of the specimen as small as 1 μm by placing an aperture in the image plane then projecting the diffraction pattern of that image onto the recording plane. Reduction of the beam diameter to a relatively small dimension makes it possible to acquire micro-diffraction patterns. The primary purpose of electron diffraction is to identify the crystal structure of the materials under investigation. Electrons are diffracted by the periodic arrangement of atoms in the crystal structure of materials, the planes in the crystal have a periodic spacing and diffract and incident electron beams through the Bragg diffraction angle \( \theta \), where the wavelength (\( \lambda \)) is \( \lambda = 2d \sin \theta \), and the spacing between the planes is \( d \).
Energy-Dispersive X-ray Spectroscopy - X-rays are produced when materials are irradiated with an electron beam. High-energy waves excite the electrons in the electron shells around the atoms in the material, causing them to jump to higher energy shells. An X-ray is then emitted as the electrons of an atom fall from their excited states to lower energy states. The wavelengths, and hence energies, of the X-rays are characteristic of the electron shell energies and the spectrum of X-rays can be used to identify different elements. In general, the fundamental emissions, which are denoted as K-α, L-α and M-α, are unique for each element. High-resolution measurements can determine the differences in composition at different positions within the matrix or an inclusion. The analysis of the energy dispersive X-ray spectrum is a very powerful technique in materials science.

3.2.5 Electron Diffraction – Interpreting the Results

Electrons may be reflected or diffracted in passing through a crystal; governed by the Bragg law. The high-energy waves interact strongly with the atoms of the crystal; therefore the penetration depth of an electron beam is around the region of 100-200 microns. An approximation of the wavelength can be obtained using the de Broglie equation:

\[
\lambda \approx 1.23 \sqrt{V}
\]

where \( V \) is the accelerating voltage.

The reciprocal space lattice is a set of imaginary points constructed in such a way that the direction of a vector from one point to another coincides with the direction of a normal to the real space planes and the separation of those points, considered as an absolute value of the vector, is equal to the reciprocal of the real interplanar distance.
Microscopy techniques applied to X100 line pipe material: Analysis

Figure 3.1 – Schematic diagram of measurements used in determining the lattice parameter, adapted from Steadman$^{37}$

Measuring the Lattice Parameter

$L = \text{Camera length and is a set constant for the TEM}$

$\lambda = \text{Wavelength of electron beam.}$

$R = \text{Measurement from diffraction pattern}$

$D = \text{Interplanar spacing}$

By comparing the two diagrams in Figure 3.1, the following equation is obtained:

$$\frac{R}{L} = \frac{1}{d} \frac{1}{\lambda}$$  \hspace{1cm} 3.2

Rearranged this gives equation 3.3:

$$d = \frac{\lambda L}{R}$$  \hspace{1cm} 3.3
To find the lattice parameter of a cubic system equation 3.4 is used:

\[ a = d \sqrt{N} \] \hspace{1cm} 3.4

where \( a \) = the lattice parameter
\( N = h^2 + k^2 + l^2 \); \( h, k \) and \( l \) are the miller indices of a set of planes.

### 3.3 Information about examined welds

Increasing length of transmission pipelines for both gas and oil has led to ever increasing costs, therefore the drive towards lighter yet stronger materials has seen a shift in momentum. Higher strength steels enable the use of thinner walled pipe, yet still enabling the same high operating pressures thus reducing both material and transportation costs. At present pipeline steels employed in transmission of gas and oils are commercially classed from X52 up to X80, these numbers relating to a given standard, increasing in strength with increasing classification number. X100 does not presently carry a commercially recognised standard though property requirements are yield strength (YTS) 700 N/mm\(^2\) and ultimate tensile strength (UTS) 770 N/mm\(^2\).

Production of the weld metal samples to be examined was done under experimental conditions at the Corus Technology Centre. Three plate types were considered, varying welding process parameters and the alloying elements found in the welding consumables. By undertaking this welding, it was hoped to gain important information as to the best welding methods to employ for this high alloy steel.

#### 3.3.1 Plate and consumable analysis

A detailed description of the plates and consumables used in the production of the three series of welds can be found in the work by Thewlis. The three plate types identified were either 12.7 mm thickness or 22 mm. The steel considered here was classed as X100 line-pipe material with major composition of carbon (C), silicon (Si), and manganese (Mn) with other additions mainly Molybdenum (Mo) and Titanium (Ti). The plate and consumables specification are presented briefly below in table 3.1 and 3.2 respectively. It is worth noting; firstly that different fluxes
were employed to ensure good running characteristics when welding the different section thicknesses, and secondly that the series 1 and 2 welds were manufactured using a 3-wire set-up, while the series 3 welds were manufactured using a 5 wire set-up.

<table>
<thead>
<tr>
<th>Weld Series</th>
<th>Plate Thickness (mm)</th>
<th>Base Analysis ≥wt.%</th>
<th>Other Additions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.7</td>
<td>0.08 C, 0.40 Si, 2.0 Mn</td>
<td>One or more of: Mo, Ni, Cu, B, Nb, V, and Ti</td>
</tr>
<tr>
<td>2</td>
<td>12.7</td>
<td>0.08 C, 1.96 Si, 2.0 Mn</td>
<td>Small additions of: Mo and Ti</td>
</tr>
<tr>
<td>3</td>
<td>22</td>
<td>0.11C, 1.95 Si, 3.01 Mn</td>
<td>Small additions of: Mo</td>
</tr>
</tbody>
</table>

**Table 3.1** – Summary of the plate analysis for that used in the production of the three series of welds manufactured for analysis of welding of X100 line-pipe material

<table>
<thead>
<tr>
<th>Weld Series</th>
<th>Welding Wire Dia.</th>
<th>Wire compositions used</th>
<th>Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4mm</td>
<td>Mn-Mo, Ni-Mo, Ti-B, Ti-Mo-B</td>
<td>Oerlikon OP107 agglomerated flux</td>
</tr>
<tr>
<td>2</td>
<td>4mm</td>
<td>Mn-Mo, Ni-Mo, Ti-B, Ti-Mo-B</td>
<td>Oerlikon OP107 agglomerated flux</td>
</tr>
<tr>
<td>3</td>
<td>4mm</td>
<td>Ti-Mo-B, Ni-Mo</td>
<td>Lincoln 995N flux</td>
</tr>
</tbody>
</table>

**Table 3.2** – Summary of the weld consumable used in the production of the three series of welds manufactured for analysis of welding of X100 line-pipe material

### 3.3.2 Weld Metal Analyses

X-ray fluorescence and wet chemical analysis were undertaken at the Corus research centre to determine the chemical composition of the weld metal as a whole. These techniques were used to determine the chemistries of the different weld beads; the degree of alloying achieved in the weld metals was defined in terms of the $P_{cm}$ formula as defined in equation 3.5. A summary of the results from analysis of the weld metal is shown in Table 3.3.
Microscopy techniques applied to X100 line pipe material: Analysis

\[ P_{cm} = C + \frac{Mn + Cr + Cu}{20} + \frac{Si}{30} + \frac{V}{10} + \frac{Ni}{60} + 5B \]

3.5

NB: Elements measured in wt.%

<table>
<thead>
<tr>
<th>Weld Series</th>
<th>( P_{cm} )</th>
<th>Mean base analysis wt.%</th>
<th>Alloying from plate and/or wire wt.%</th>
<th>Weldment oxygen content %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.218-0.250</td>
<td>0.065 C, 2.04 Mn, 0.53 Si, 0.0052 N</td>
<td>0.21-0.72 Ni, 0.24-0.51 Mo, 0.24 Cu, 0.010-0.0025 B, 0.035 V, 0.032-0.034 Nb, 0.008-0.022 Ti</td>
<td>0.0285-0.0335</td>
</tr>
<tr>
<td>2</td>
<td>0.260-0.288</td>
<td>0.071 C, 2.28 Mn, 1.54 Si, 0.0054 N</td>
<td>0.65-0.66 Ni, 0.21-0.23 Mo, 0.0011-0.0025 B, 0.012-0.020 Ti</td>
<td>0.0240-0.0270</td>
</tr>
<tr>
<td>3</td>
<td>0.305-0.313</td>
<td>0.083 C, 2.74 Mn, 1.36 Si, 0.0056 N</td>
<td>0.35 Mo, 0.0025-0.0027 B, 0.010-0.019 Ti, one deposit 0.74 Ni</td>
<td>0.0220-0.0280</td>
</tr>
</tbody>
</table>

Table 3.3 – Summary of the findings of the weld metal analysis using x-ray and wet metal techniques for the three series of welds to be examined.

3.3.3 Representative examples for examination

From the three series of welds produced an example from each set was selected for examination. These welds were selected at random as typical examples of what could be found in the three distinct series. A summary of the individual weld metal analyses, for each weld to be examined, can be found in Table 3.4.
Table 3.4 – Summary of the weld analysis for the three individual welds selected for examination

3.4 Light microscopy examination of X100 welds

The three samples chosen representing the 3 different series of welds were examined on the optical microscope, a Reichert-Jung MeF3, prior to examination on the TEM. The samples were ground then polished to 0.25μm, on a Struers DAP-U polishing wheel, using diamond paste. The samples were then etched using a 2% nital solution.

3.4.1 Series 1 Welds

Images were taken at magnifications from 2x through to 100x magnification. In Figure 3.2 examples of the acicular ferrite microstructure are shown, taken at 100x magnification, highlighting the chaotic structure endemic to this particular microstructure. Throughout the samples it is seen that this acicular ferrite structure nucleates from inclusions; Figure 3.2(b) shows this acicular ferrite nucleating from relatively large round inclusions, when compared to the acicular ferrite lath size.
High volume fractions of acicular ferrite (96.4-99.5%) were found with observations of residual quantities of austenite grain boundary primary ferrite, ferrite side-plate and intragranular ferrite plates. These measurements are found through a technique known as point counting, where a grid is moved randomly over the specimen being examined and the microstructure found under the interconnecting points of the grid is counted. It is usual to take 1000 points and then present the volume fraction of each phase as a percentage. Large inclusions were present (4-5 μm),
generally surrounded by fine acicular ferrite. This acicular ferrite is notably very fine, particularly in the Ti-B alloyed deposits, grain sizes measured at between (1-2 $\mu$m).

### 3.4.2 Series 2 Welds

The volume fraction of acicular ferrite was found to be smaller than in series 1 welds, 79.1-90.0%. Primary ferrite was found to vary between 1.5-6.0%, whilst ferrite side-plate volume fraction varied between 6.2-12.8%. This gave the microstructure appearance of large ferrite plates interspersed with acicular ferrite, with regions of continuous acicular ferrite also present. These large laths of acicular ferrite are seen in Figure 3.3(a) surrounded by a finer acicular ferrite matrix, while in Figure 3.3(b) the nucleation of these acicular ferrite microstructures are seen to nucleate from inclusions as seen in the series 1 weld.

**Figure 3.3(a)** - Series 2 weld showing long laths of ferrite surrounded by a finer acicular ferrite matrix
3.4.3 Series 3 Welds

The level of acicular ferrite present in the series 3 welds was low; a volume fraction of between 55.4-64.6% was recorded. Primary ferrite was also observed to be low, with a recorded volume fraction of between 0.8-1.7%. Ferrite side-plate, volume fraction 28.6-31.3% and martensite/austenite volume fraction 3.4-10.7% were high. The intragranular regions generally showed large ferrite plates, these apparently being nucleated on big inclusions, interspersed with martensite and retained austenite. Examples of these long laths ferrite side-plate are seen in Figure 3.4(a), round inclusions are seen to be nucleating sites for these laths. Figure 3.4(b) shows the fine ferrite matrix of acicular ferrite with large regions of aligned ferrite side-plate. Thewlis\textsuperscript{22} comments as to the difficulty in distinguishing between the acicular ferrite and non-aligned ferrite side-plates which could lead to over-estimation of the acicular ferrite content and therefore the figures proposed are approximations.
3.5 Previous Work on X100 Line-pipe

From the work carried out by G. Thewlis\textsuperscript{22}, of Corus, on the X100 pipe being investigated here various points came to light. The work concluded that optimum strength and toughness is obtained in Ti-Mo-B alloyed weld metals, with measured $P_{\text{cm}}$ values measured at between 0.218-0.250. These optimised weld metal microstructures show over 97% acicular ferrite, with less
than 2% grain boundary primary ferrite. The X100 was found to transform at significantly lower
temperatures than those reported with X65 pipe, during thermal cycling and cooling at typical
weld cooling rates. X65 plate deposits are found to contain acicular ferrite in the form of
idiomorphic primary ferrite and intragranular Widmanstätten ferrite.

The maximum transformation in these optimised welds was found to occur at temperatures
between 515-570°C\textsuperscript{22}, this is indicative of the fact that acicular ferrite in these welds is found in
the form of Widmanstätten ferrite and/or bainite. The more highly alloyed weld metals
containing 2-3% Mn and 1.5% Si transform at low temperatures and show increased strength,
with a substantial loss of toughness. This can be attributed to the relatively unimpeded growth of
large ferrite plates from big inclusions and the replacement of ultra fine acicular ferrite between
these plates by blocks of martensite and austenite. The findings were applied practically to one
pass per side submerged arc welds manufactured to the optimum weld metal chemistry. This
confirmed the applicability of the optimised weld metal compositions for thin section X100 line-
pipe.

3.6 TEM analysis of series 1, 2 and 3 welds

TEM specimens must be electron transparent and representative of the material one wants to
study. In most cases it is desirable to have specimens that are uniformly thin, stable under the
electron beam, conducting and non-magnetic. There are many ways to prepare specimens for
TEM. The chosen method will depend on both the type of material and the information one
needs to obtain. The most important aspect to bear in mind is that the preparation technique must
never affect what one observes or measures. Thin foils were cut from the bulk sample using a
Struers Accutom 5 circular saw, using a 356 blade. The 356 blades are for use with ferrous
metals with $H_v$ 350-800, the blade is a Bakelite $\text{Al}_2\text{O}_3$ compound. The thin foils were then cut to
3mm diameter discs using a spark eroder. Grinding follows this process; on 800 grit paper to
bring the samples down to a thickness less than 100\(\mu\text{m}\). The samples are polished using a 5%
perchloric mixture in methanol at $-50^\circ\text{C}$, using a Struers Tenapol-3 polishing cell. Washing is
required in two consecutive baths of methanol to prevent any further surface reaction with
residual polishing solution, before drying ready for use in the TEM. It was found that without
due care in the storing of these samples an oxide layer built up on the sample surface making it
harder for good penetration of the electron beam.
The majority of the TEM work on all three series, apart from the inclusion work done on the series 1 weld, was carried out on the JEOL 100CX TEM. Diffraction patterns taken from inclusions using thin foils of the series 1 weld sample were obtained using the JEOL 2000 FX TEM. This machine utilises a higher accelerating voltage in the electron beam, 200 kV. This higher accelerating voltage was required due to problems with magnetism and penetration through thick inclusions and allowed the simultaneous analysis by EDX and by use of diffraction patterns.

3.6.1 TEM analysis strategy

In an effort to understand the metallurgy of the weld metal microstructure, it was decided to follow up the use of optical microscopy techniques by utilising transmission electron microscopy (TEM) techniques to analyse the characteristics of the inclusions and nucleating ferrite matrix. When analysing the steel welds efforts were concentrated on the nucleation sites to see whether the orientation and chemical make-up are in any way a cause for better nucleation of larger laths or fine acicular ferrite. This would give an insight as to whether there were any difference between inclusions seen to nucleate acicular ferrite and those seen to act as nucleation sites for the long ferrite laths. Diffraction patterns were taken both on inclusions and around inclusions to get a picture of the type of matrix that is seen. These diffraction patterns were backed by EDX analysis, breaking down the approximate chemical analysis of inclusions, in an attempt to get a full picture of what is happening. All figures referred to in this section can be found at the end of the chapter in order of weld series.

Work by Blais et al\textsuperscript{18}, has shown that the formation of MnTi\textsubscript{2}O\textsubscript{4} on the surface of inclusions is common in high concentration Ti welds. This compound is a very efficient nucleant for of acicular ferrite. It is also argued that the formation of TiO, TiO\textsubscript{2}, and TiO\textsubscript{3} is unlikely on the outer surface of an inclusion due to the high melting points, and that MnTi\textsubscript{2}O\textsubscript{4} is formed in preference having a lower melting point due to the combination with another mono-oxide MnO. Other compounds that can be found in the inclusions are galaxite MnAl\textsubscript{2}O\textsubscript{4}, manganese sulphide MnS, and aluminium oxide Al\textsubscript{2}O\textsubscript{3}. The intention of the TEM work was therefore to relate the inclusions present to observations from the literature.
3.6.2 Comparison of EDX Analysis on Inclusions Present in Series 1, 2 and 3 Welds.

In comparing the results of EDX on all three series of welds, there is a noticeable difference in the chemical make-up of the inclusions present, as a function of the levels of titanium present, Table 3.3. From the various spectra taken, it can be seen that Al, Si, Ti and Mn are the main elements found in differing quantities within inclusions. EDX analysis was applied at the edge and at the centre of inclusions, as it was expected that the chemistries of edge and centre would differ as a result of segregation during solidification.

Titanium is found in a relatively larger quantity in the centre of inclusions, when compared with the outer shell of inclusions in the series 2 weld, see Figure 3.12 (a). There is a differing case found for the series 1 weld; EDX results found in Figure 3.9, show titanium is the dominant element from this analysis, though in Figure 3.7 we see that there is a relatively larger titanium presence in the centre of the inclusion. This suggests that there is a titanium oxide shell, TiO, TiO\(_2\) or TiO\(_3\), when titanium is found in greater quantities at the edge. Though where lower levels of titanium are input to the welding process, the surface of inclusions is more likely to be of the form MnTi\(_2\)O\(_4\), as this has a lower solidification temperature. This would mean that the core of these inclusions would probably take a Ti\(_x\) form, with titanium being present in higher concentration in the centre of inclusions.

Examination of inclusions found in the series 3 weld showed a mixture of chemistries containing little or no titanium compared with other alloying elements. Inclusions found in the series 3 weld contained higher levels of Mn, Al and Si. The inclusion chemistries being either alumina (Al\(_2\)O\(_3\)) or galaxite (MnAl\(_2\)O\(_4\)) with some silicates present. EDX analysis of the series 3 weld inclusions can be seen in Figure 3.18(a) and Figure 3.19, showing an inclusion containing relatively small amounts of titanium and no titanium respectively.

From the wet analysis of the weld samples taken into consideration here, found in Table 3.4 (a – c), it is observed that levels of the important alloying elements are present in the weld in general. This can be compared with EDX data to see whether findings would be expected. From these data, it is seen that levels of titanium drop from Series 1 – 3, this coincides with a drop in the volume fraction in acicular ferrite. The titanium rich outer shell of inclusions is also only found
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in series 1 welds, suggesting that these inclusions are better nucleation sites for fine acicular ferrite.

With increasing series number, an increase in the volume fraction of Mn (Manganese) is seen, this suggests that there is more scope for the presence of MnTi$_2$O$_4$ in these welds. A decrease in the volume fraction of fine acicular ferrite is observed with increase in the volume fraction of Mn, there is a case to argue with the findings of Blais et al$^{38}$, finding Titanium rich welds (TiO, TiO$_2$ and TiO$_3$ rich) more likely to promote acicular ferrite.

Galaxite is another possible compound found as inclusions in these welds. Galaxite is a member of the spinel series, with a formula of (Mn,Fe$^{2+}$,Mg)(Al,Fe$^{3+}$)$_2$O$_4$. However, galaxite is known as the manganese member of the spinel series, and when pure its formula is MnAl$_2$O$_4$. Galaxite is found to be FCC in structure; this will make identification of this type of inclusion quite easy as the majority are found to be of a BCC structure type. A typical FCC structure found in an inclusion can be seen in Figure 3.11.

In the work of Thewlis et al$^{39}$ the misfit between various substrates and ferrite are calculated, the relevant inclusion types are summarised in Table 3.5. The calculations do not take into account lattice expansion effects during the $\gamma \rightarrow \alpha$ transformation temperature and ambient temperature as these are of negligible magnitude. The work concluded that low misfit is an important factor in influencing the formation of large volume fractions of acicular ferrite, along with the volume fraction and size distribution of inclusions.
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<table>
<thead>
<tr>
<th>Ferrite</th>
<th>Substrate</th>
<th>TiO</th>
<th>Alumina</th>
<th>Galaxite</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>100</td>
<td>3.0</td>
<td>3.2</td>
<td>1.8</td>
</tr>
<tr>
<td>100</td>
<td>110</td>
<td>22.0</td>
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<td>20.5</td>
</tr>
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<td>110</td>
<td>100</td>
<td>24.4</td>
<td>19.0</td>
<td>22.8</td>
</tr>
<tr>
<td>100</td>
<td>110</td>
<td>37.4</td>
<td>33.3</td>
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<td>100</td>
<td>110</td>
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</tr>
<tr>
<td>100</td>
<td>111</td>
<td>34.5</td>
<td>28.5</td>
<td>32.8</td>
</tr>
<tr>
<td>110</td>
<td>111</td>
<td>15.9</td>
<td>11.0</td>
<td>14.4</td>
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<tr>
<td>111</td>
<td>100</td>
<td>20.8</td>
<td>23.6</td>
<td>20.9</td>
</tr>
</tbody>
</table>

Table 3.5 – Results of diffraction pattern analysis of inclusions found in the three series of welds examined in this chapter, alongside the amount of misfit present sourced from Mills et al.39

3.6.3 Diffraction pattern analysis of inclusions

Diffraction patterns were taken both from inclusions, and from grains seen to nucleate from inclusions. This allowed for the identification of the kind of structure present, it was also possible to gain information on the lattice parameter, and the orientation of the crystal structure, and comparison of misfit.

Problems were encountered when taking diffraction patterns from inclusions, using thin foils. The samples were ferritic and hence magnetic, this lead to problems in getting a clear image due to the magnetic field distorting the image by causing a pulling effect on the electron beam. Interference from the matrix caused overlapping of patterns so making it difficult to interpret the
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results taken by diffraction patterns. A solution to this would be to take carbon replicas, thus extracting the inclusions, however as some of the inclusions are large care would be need to be taken to ensure that all sizes of inclusions were extracted.

The thickness of the inclusions present was also a problem; this meant that in the case of the series 1 welds the samples had to be examined with a TEM of higher voltage to enable sufficient penetration of the samples. An example of a thick inclusion can be seen in Figure 3.6, the diffraction pattern is unclear and therefore impossible to interpret. A solution to this would be ion beam thinning of the samples to a thickness more suitable to penetration of an electron beam.

Results obtained from diffraction patterns taken from inclusions, show the majority of inclusions to be BCC structured, though a small portion are found to be FCC structured. This leads to the consideration of spinels being present, one example being galaxite. In Figure 3.11 an example of a FCC structured inclusion is shown, these structures have a larger lattice parameter than that of BCC structured inclusions. The example shown in Figure 3.11 has a lattice parameter of 11.525 Å, with an orientation of [1 2 3]. Comparing this with the relative BCC structured inclusion found in the series 1 weld, seen in Figure 3.8 we find a lattice parameter of 9.25Å, with an orientation [013].

In Figure 3.16 and Figure 3.17 we can see a comparison in the different shaped inclusions encountered in the welds examined. These two examples were taken from a series 3-weld sample. In Figure 3.16 there are many holes in the matrix surrounding the main inclusion in the picture, these holes are where smaller inclusions have fallen out during electro-polishing of the surface. The non-round inclusion found in Figure 3.17 has an orientation of [0 1 1], being a bcc structure, and has a lattice parameter of 3.221Å smaller than that found in round inclusions showing the same bcc structure, seen in Figure 3.8.

In Figure 3.18(b) an example of a round inclusion found in a series 3 weld sample is seen, it is observed that the inclusions are agglomerated. These inclusions have low titanium content, as can be seen in the EDX analysis shown in Figure 3.18(a).
3.6.4 Diffraction pattern analysis on the metal matrix

The matrix analysis was mainly concerned with nucleating grains around inclusions, though some additional diffraction patterns were taken on points of interest in the matrix, for example the micro-laths found in Figure 3.15. These laths showed an \([011]\) orientation, with a lattice parameter of 4.856 Å. The interesting feature of these laths is the smaller laths seen to grow across the laths normally seen through the light microscope. Analysis of the matrix through series 1, 2 and 3 gave consistent results, showing a BCC structure throughout.

<table>
<thead>
<tr>
<th>Weld Series</th>
<th>Grain Number</th>
<th>Lattice Parameter</th>
<th>Orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2.869</td>
<td>[T13]</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.869</td>
<td>[012]</td>
</tr>
<tr>
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<td>1</td>
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<td>[011]</td>
</tr>
<tr>
<td></td>
<td>2</td>
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<td>[T13]</td>
</tr>
<tr>
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<td>2.869</td>
<td>[T13]</td>
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<td>2.916</td>
<td>[T11]</td>
</tr>
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<td>2</td>
<td>4.856</td>
<td>[011]</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Table 3.6 – Results of Diffraction Pattern Analysis of Weld Matrix for Series 1, 2 and 3 Welds.

In Table 3.6, the lattice parameter is unchanged for the majority of grains measured, independent of the alloying content (weld series). A high level of orientation in grains around an inclusion can be seen, as in the case of the series 2 weld, three out of the four grains examined followed a degree of orientation in the same plane. In Figure 3.5 we have an example of a series 1 weld, with diffraction patterns taken from two grains, seen to nucleate from the inclusion. The lattice parameter is measured at 2.869 Å, the orientation of the crystal structure is found to differ, but both have a bcc structure. Similar results to those obtained from the series 1 weld sample were found in the series 2 weld sample, shown in Figure 3.10. The lattice parameter of the series 2 weld sample was measured at 2.869 Å with 3 out of 4 grains showing the same orientation, [T13]; the crystal structure of the matrix is bcc. This high orientation of the grains suggests that the grains are nucleating from the inclusion. The series 3-weld sample in Figure 3.14 showed a
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different pattern to the series 1 and 2 weld samples. The grains measured showed differing lattice parameters and orientation, though both were of a bcc crystal structure.

EDX analysis undertaken on matrix samples has shown that the welds have a high concentration of ferrite, showing an average 96% Fe constituent. The typical breakdown of the matrix composition can be seen in Table 3.7, the full results from the EDX analysis of the matrix can be found in appendix I.

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Fe</th>
<th>Si</th>
<th>Ni</th>
<th>Mn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Wt.%</td>
<td>96.0</td>
<td>1.5</td>
<td>0.6</td>
<td>1.9</td>
</tr>
</tbody>
</table>

Table 3.7 – Average Wt.% for Typical Weld Matrix EDX Analysis

3.6.5 Discussion

It is well recognised throughout the literature that acicular ferrite formation in weld metals depends on retarding the nucleation and growth of ferrite at the austenite grain boundaries, whilst creating a high degree of nucleation at inclusions and dislocations in the intragranular regions, covered in great detail by Thewlis\textsuperscript{22, 39, 40, 41}.

Investigation of the three series of welds has shown that with decreasing concentration of titanium and increasing concentration of Mn, Al and Si the inclusion chemistries move from a TiO\textsubscript{x} form to more complex oxides and silicates of the manganese and aluminium. The work of Blais et al\textsuperscript{38} puts forward explanations as to the formation of these inclusions, containing substrates with high solidification temperatures at the core with surface coatings of substrates having lower solidification temperatures. This work suggests the need for oxides of titanium on the periphery of inclusions for good promotion of acicular ferrite. From the examination of the EDX analysis of the inclusions found in the three series of welds, the surface chemistry of inclusions is seen to differ with decreasing titanium content and increasing other alloying elements. In series 1, containing highest levels of titanium and lowest levels of Mn, Al and Si. Inclusions are seen to contain a high level of Ti in both core and surface layers. This suggests that the surface chemistry will take the form of TiO\textsubscript{x}, with the possibility of some Mn-Ti...
substrates present. With the high levels of acicular ferrite present and the TiO\textsubscript{x} inclusions, the findings agree strongly with what is found within the literature.

Examination of series 2 welds containing a relatively smaller amount of titanium, showed that inclusions were most likely to have surface chemistry of the form MnTi\textsubscript{2}O\textsubscript{4}. Given that Ti was still present, they also had a strong ability to promote acicular ferrite growth, although not as strong as TiO\textsubscript{x} chemistries. The series 3 welds, having the lowest titanium levels, and the smallest volume fraction of acicular ferrite were found to have little or no titanium in inclusions examined. Inclusions in series 1 welds would probably take the form of alumina (Al\textsubscript{2}O\textsubscript{3}), galaxite (MnAl\textsubscript{2}O\textsubscript{4}), MnS or silicates, although no Si rich inclusions were found and silicon is normally found in large quantities in the welding slag. With the lower levels of fine acicular ferrite and increased number of long ferrite laths, it can be presumed that these inclusions types do not have the same ability to promote acicular ferrite growth. Where titanium is present in series 3 welds, it is most probably in the form of MnTi\textsubscript{2}O\textsubscript{4}, which solidifies before the manganese and silicon rich inclusions so that it is no longer in contact with the ferrite matrix, and therefore is not able to promote growth of acicular ferrite.

Several pieces of literature discuss the relationship between misfit of the matrix and inclusions speculating on the degree of misfit and the promotion of different ferrite structures. Both Thewlis et al\textsuperscript{39} and Blais et al\textsuperscript{38} make reference to the work of Bramfit\textsuperscript{42} and the use of Bain orientation for determination of misfit and promotion of acicular ferrite through a mechanism determined by lattice matching.

Low misfit between inclusions and ferrite matrix is thought to be highly influential in the promotion of acicular ferrite growth. Both galaxite and TiO\textsubscript{x} inclusions are seen to have low misfit values, shown in Table 3.5, though TiO\textsubscript{x} inclusions are especially effective because of the number of particles that are present on the surface of inclusions. The nucleation process being independent of the underlying bulk of the inclusion composition.
3.6.6 TEM analysis images and EDX analysis graphs

**Figure 3.5** - Diffraction patterns taken around an inclusion to determine orientation of nucleating grains. Series 1 weld

**Fig 3.6** - Diffraction pattern from a typical inclusion found in a series 1 weld. BCC structure
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Figure 3.7 – EDX analysis results from the centre (a) and edge (b) of the inclusion in Figure 3.6

Figure 3.8 - Diffraction pattern from a typical inclusion found in a series 1. BCC structure
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**Figure 3.9** - EDX analysis results from the centre (a) and edge (b) of the inclusion in Figure 3.8

**Figure 3.10** - Diffraction patterns taken around an inclusion to determine orientation of nucleating grains Series 2 weld
Figure 3.11 – Diffraction pattern from a typical inclusion found in a series 2 weld - FCC structure

Figure 3.12(a) – EDX analysis of a titanium rich inclusion in a series 2 weld
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**Figure 3.12(b)** – Image of inclusion examined in Figure 3.11 (a)

**Figure 3.13 (a)** – EDX analysis of an inclusion shell from a series 2 weld
Figure 3.13 (b) – EDX analysis of inclusion centre from a series 2 weld

Figure 3.13 (c) - Image of inclusion examined in Figure 3.13 (a) and (b)
Figure 3.14 – Diffraction patterns taken around an inclusion to determine orientation of nucleating grains - Series 3 weld

Figure 3.15 – Micro-laths found within laths in the microstructure of a series 3 weld. BCC structure
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Figure 3.16 - Diffraction pattern from a typical round inclusion found in a series 3 weld

Figure 3.17 – Diffraction pattern from a non-round shaped inclusion in a series 3 weld
Figure 3.18 (a) — EDX analysis of inclusion containing titanium from a series 3 weld

Figure 3.18 (b) — Image of inclusion examined in Figure 3.18 (a)
Figure 3.19 – EDX Analysis of an Inclusion Containing no Titanium from a Series 3 Weld.
3.7 Conclusions

- A definite increase in volume fraction of large lath size ferrite plates has been seen with increasing weld series number, this being relative to the levels of alloying elements present in the welds, in particular Ti and B.

- It is difficult to distinguish acicular ferrite laths from unaligned ferrite sideplate in the series 3 welds.

- TEM results, using diffraction pattern and EDX analysis, have shown that there is no significant difference in the matrix structure found in any of the weld series. Chemical composition and crystal structure show no significant differences, with all measurements taken showing the crystal structure to be BCC as expected, with no significant content of retained austenite.

- As the ferrite matrix does not seem to change through the series, although inclusion chemistry does change through the series, growth of ferrite laths, and nucleation and volume fraction of acicular ferrite is linked to inclusion chemistry. The formation of differing shell and centre compounds being a major contributor to the promotion of acicular ferrite.

- Both FCC and BCC inclusions are present in the welds, which contain different chemistries. There is a distinct difference between inclusion centres and outer shells, showing that certain acicular ferrite promoting compounds are present on the inclusion surfaces.

- Ti rich inclusions are seen to be good nucleation sites for acicular ferrite microstructure, while Mn and Al rich inclusions are seen to be strong nucleation sites for the long ferrite laths. This is due to misfit between inclusion surface and ferrite matrix, low misfit being required for promotion of acicular ferrite growth. TiO$_x$ inclusions are seen to have low misfit values with the ferrite matrix, this is also seen for galaxite (MnAl$_2$O$_4$), though TiO$_x$ inclusion surfaces contain a higher number of particles thus creating a better chance of nucleation.
- High concentration Ti welds, such as the series 1 welds, are more likely to contain inclusions containing TiO$_2$, TiO$_3$ and TiO centres, with MnTi$_2$O$_4$ surface in series 2 welds where manganese content is relatively high, and a decrease in titanium is noticed.

- Series 2 and 3 welds having a lower Ti concentration and will contain more alumina (Al$_2$O$_3$) and galaxite (MnAl$_2$O$_4$) inclusions, with the possibility of manganese sulphide forming dependent on the level of sulphur impurity in the steels.
3.8 Chapter Summary

Three series of welds have been investigated in this chapter, these welds being made using three different plate types that could be classed as X100 line-pipe material. The welds examined were produced using various combinations of allowing elements manipulated through the use of a variety of welding wires, flux and alloying metal powders. The purpose of the manufacture of these welds was to determine a suitable welding procedure specification for such high alloy steel. Research into these welds was initially carried out at the Corus research centre in Rotherham, taking into account optical microscopy, X-ray and wet analysis techniques. The aim of this chapter was to firstly enable the author to get some hands on knowledge of the metallurgy involved in the welding of line-pipe steels, and also to gather some more detailed data on the microstructure seen in these welds.

Three welds were chosen for examination, one from each welding series, these were initially evaluated using optical microscopy. Point counting techniques were employed to determine the volume fraction of each particular phase present. This evaluation showed a decrease in fine acicular ferrite and an increase in large ferrite laths with decreasing titanium content, and increasing silicon and manganese content. The large ferrite laths seen in the optical microscopy work, seemed to be nucleating from large round inclusions and therefore this led on to closer examination through TEM techniques.

TEM techniques were employed to closely investigate the chemical make-up and crystallography of both the inclusions seen to act as nucleation sites and the ferrite plates nucleating from them. Results of this work showed the ferrite matrix to have no significant change throughout the three series of welds, with all plates having a BCC structure with not much variation in the orientation of these crystals. Investigation of the inclusions showed a variety of results, with a decrease in the titanium (Ti) rich inclusions coming with decrease in Ti input to the welding procedure. Where Ti rich inclusions were in small number they were replaced with aluminium (Al) and manganese (Mn) rich inclusions, seen to be the nucleating sites for the large ferrite plates, whilst the Ti rich inclusions showed to be inclusion sites for the finer acicular ferrite structures.

The literature review in this chapter has also made an attempt to cover methods used investigating the effects of the welding on the steel microstructure. Theory behind the optical and
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electron microscopes details the techniques used in this to investigate the microstructural characteristics of X100 welds. Covering the theory behind the types of imaging techniques used, and methods of determining the orientation of the crystal structure of the weld metal.
Chapter 4 – Neural networks – Introduction to the modelling techniques and application: Literature

4.1 Introduction

There are many problems in physical metallurgy for which it is difficult to develop a first principles scientific model due to their complexity. One particular example is in the area of multi-wire submerged-arc welding, where there are a large number of variables including heat input, welding speed, number of wires, electrode stick-out and spacing, number of passes, and compositions of the flux, wire and plate. Properties of the final weld may therefore be difficult to predict, especially quantities such as weld metal toughness, which are known to be dependent on many factors. This means that for multi-wire submerged-arc welding processes, the choice of plate and consumable chemistry and welding conditions to meet contract requirements is often by reference to previous experience or exhaustive experimental trials. A predictive model, therefore, is a useful tool in the quantification of this approach to plate and consumable choice, with desired outputs being typically weld metal composition, microstructure and properties.

One useful modelling technique for such complex problems is neural networks. A neural network is an artificial representation of the human brain that tries to simulate its learning process. The term "artificial" means that neural networks are implemented in computer programs that are able to handle the large number of necessary calculations during the learning process. The first models were based upon medical knowledge of how the different parts of the brain were interconnected. Through time more sophisticated models have been developed, which additionally consider probabilistic methods to model characteristics of the brain such as uncertainty and logical representation of knowledge. Nowadays, there is a wide range of neural network based techniques and commercial software packages available for use in the modelling of data. The aim of this literature survey is to consider previous work in areas concerned with the application of neural network modelling to welding and other areas of metallurgy.
4.1.1 What is a neural network?

Neural networks have been described in a variety of ways in the literature.

"... a neural network is a system composed of many simple processing elements operating in parallel whose function is determined by network structure, connection strengths, and the processing performed at computing elements or nodes."8

"A neural network is a massively parallel distributed processor that has a natural propensity for storing experiential knowledge and making it available for use. It resembles the brain in two respects:

1. Knowledge is acquired by the network through a learning process.
2. Inter-neuron connection strengths known as synaptic weights are used to store the knowledge."43

Neural networks can be considered to be powerful tools, designed to mimic the human brain, in that they can recognise patterns and draw conclusions when presented with complex, noisy and irrelevant information. The neural network is made up from several simple processing units, these are known as nodes, being arranged in a pattern following those of a biological network. These nodes are inter-connected by weighted connections; the weights being adapted during the learning process to best improve the performance of the network. The net architecture, node characteristics and the training rules specify each neural network. The rules obtained from the process of training determine the rules and algorithms necessary to enhance the performance of the network.

Neural networks have been applied to an increasing number of real-world problems of considerable complexity. Their most important advantage is in solving problems that are too complex for conventional technologies, for example, problems that do not have an algorithmic solution or for which an algorithmic solution is too complex to be found. In general, because of their abstraction from the biological brain, neural networks are well suited to problems that people are good at solving, but for which computers are not. These problems include pattern recognition and forecasting, which requires the recognition of trends in data.
4.1.2 Why use a Neural Network?

Neural networks, with their remarkable ability to derive meaning from complicated or imprecise data, can be used to extract patterns and detect trends that are too complex to be noticed by either humans or other computer techniques. A trained neural network can be thought of as an "expert" in the category of information it has been given to analyse. This expert can then be used to provide projections given new situations of interest and answer "what if.....?" questions. Other advantages include adaptive learning abilities, self-organisation, real-time operation and parallel computation.

4.2 Development within the Field of Neural Network Modelling

Biological computation of the brain is so effective that it would seem obvious that similar properties may be obtained by building models based upon the same principles. The major points to be considered are large numbers of highly inter-connected processing nodes, adaptable connections and parallel processing.

Relatively simple models, when compared to a biological neural network, have been built but researchers have a number of difficulties. The largest is the high complexity of biological neurons; neurons receive and send stimuli thus transmitting patterns of pulse-like activity through the complex network of neurons in the brain. When a neuron is active, output is produced in pulse form that travels along paths called axons, to the receivers, called dendrites via an inter-connection called a synapse seen in the layout of a neuron, Figure 4.1. Actual output sent from one neuron to another is dependent upon weighting factors, and therefore determines the effect of the output upon the receiving neuron. For example if two neurons were to be only weakly connected, by association, the potential output will be scaled down, the proportion of the output adjusted by the weight of the connection.
4.2.1 Brief History

Initially simulations using formal logic were developed, McCulloch and Pitts (1943)\textsuperscript{45} created neural networks based on their understanding of neurology. Another attempt, this time using computer simulations was carried out by two groups (Farley and Clark, 1954\textsuperscript{4}; Rochester, Holland, Haibit and Duda, 1956\textsuperscript{5}). The first group (IBM researchers) maintained close communication with neuroscientists during development.

Not only was neuroscience influential in the development of neural networks, but psychologists and engineers also contributed to the progress of neural network simulations. Rosenblatt (1958)\textsuperscript{6} stirred considerable interest and activity in the field when he designed and developed the Perceptron. A major influence of the work came from Donald Hebb\textsuperscript{47}, who in 1949 expressed an idea, known as Hebbian learning that enabled the development of learning rules that could be used when working with neural networks.

In 1969 Minsky and Papert wrote a book in which they generalised the limitations of single layer Perceptrons to multi-layered systems\textsuperscript{7}. In the book they said "...our intuitive judgement that the extension (to multi-layer systems) is sterile". The significant result of their book was to dampen interest for research into neural network simulations for some years.
Developments over the past 20 years have seen various approaches to the evolution of neural networks. Major influences have come from Grossberg and Carpenter, with their resonating algorithms, better known as ART (Adaptive Resonance Theory). Kohonen developed associative techniques, and Klopf developed a basis for learning in artificial neurons based on a biological principle for neuronal learning. The back-propagation learning method was developed by Werbos, however several years passed before this approach was popularised. Amari was involved with theoretical developments; he published a paper that established a mathematical theory for a learning basis, while Fukushima developed a step-wise trained multi-layered neural network for interpretation of hand-written characters.

4.3 Network architecture and operation

The activity of the input units represents the raw information that is fed into the network. The activity of each hidden unit is determined by the activities of the input units and the weights on the connections between the input and the hidden units, similarly between hidden units and output units. Within this type of network the hidden units are free to construct their own representations of the input. The weights between layers of units determine when each node is active, and so by modifying these weights, a node can determine what it represents. A typical neural network architecture is shown in Figure 4.3, containing two inputs, 4 nodes in the hidden layer, and a single output. Increasing the number of units in the model, in particular the number of hidden units will make a more complex model with a considerable number of parameters to be determined.

Single-layer and multi-layer architectures are also distinguishable. The single-layer organisation constitutes the most general case and is of more potential computational power than hierarchically structured multi-layer organisations. In multi-layer networks, units are often numbered by layer, rather than using a global numbering.

4.3.1 Simplicity – Occam’s Razor

The principle that we should prefer simple models to complex models when the latter are not necessary to explain the data is often held to be an essential component in neural network design. Simplicity can be achieved by adhering to Occam’s razor (otherwise known as Ockham’s razor),
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a principle attributed to the 14th century logician and Franciscan friar, William of Ockham. Much can be found out about William Ockham throughout philosophical literature; one such example is by McGrade\textsuperscript{52}.

The principle states "entities should not be multiplied unnecessarily." Many scientists have adopted or reinvented Occam's razor as in Leibniz's "identity of observables". Also Isaac Newton stated the rule: "We are to admit no more causes of natural things than such as are both true and sufficient to explain their appearances." The most useful statement of the principle for scientists is, "when you have two competing theories which make exactly the same predictions, the one that is simpler is the better." Throughout the literature references to the simplicity rule are found, and applied to the construction of neural network models and their application to real world situations. Neal discusses the notion of limiting the complexity of models, and the meaning and utility of Occam's razor within the Bayesian framework of a neural network\textsuperscript{53}.

4.3.2 Data Flow

Feed-forward neural networks allow signals to travel in one direction only, from input to output. There are no feedback loops; therefore the output of any layer does not affect that same layer or previous layers. Feed-forward neural networks tend to be straightforward networks that associate inputs with outputs, being extensively used in pattern recognition. This type of organisation is also referred to as 'bottom-up' or 'top-down'. The network in Figure 4.3 is fully connected; every node is connected with every node in the next layer and with the unit in the output layer. This type of neural network model is used throughout the work described in this thesis. The units in the hidden layer are responsible for the non-linearity of the net.

Feedback networks allow signals to travel in both directions by introducing loops in the network. Feedback networks are very powerful and can become extremely complicated. Feedback networks are dynamic; their 'state' is changing continuously until equilibrium is reached. They remain at the equilibrium point until the input changes and a new equilibrium needs to be found. Feedback techniques are most popular when considering the training of a model. This is due to the ability of the model to correct itself, thus producing a highly accurate predictive tool.

4.3.3 Feed Forward Neural Network Model
In order to explain how the feed-forward model works, a mathematical representation of the architecture in Figure 4.3 is required. The function that maps inputs, \( \vec{i} \), and the output, \( \sigma \), must be defined (to simplify the explanation a single input will be considered). This mapping function \( \sigma = f(\vec{i}, \theta) \) can be expressed as:

\[
\sigma(\vec{i}, \theta) = b^{(o)} + \sum_k \omega_k^{(o)} i_k + \sum_l \omega_l^{(h)} f_l
\]

\[
f_l = \tanh(h_l)
\]

4.1

\[
h_l = b_l^{(h)} + \sum_k \omega_{k,l}^{(h)} i_k
\]

where the weights \( \omega \) and biases \( b \) are the parameters of the net. The parameter vector \( \theta \) of the net is made up of the weights \( \omega \) and biases \( b \). The input layer merely distributes the input, \( \vec{i} \), onto the hidden layer. The first changes to the input data are undertaken in the hidden layer. Input to the \( k \) node in the input layer is represented as a vector \( \vec{i} \), the vector components being \( i_k \) (\( k = 1 \) to \( n \)); nodes on the hidden layer are represented as the \( l \) node. A corresponding weight, \( \omega_{k,l}^{(h)} \), is multiplied with the input and an internal bias, \( b_l^{(h)} \), added to every input. The transfer function on the hidden units is a function of the weighted total input sum plus the internal bias, \( h_l \).

4.3.4 Transfer Function

The activation function is a non-linear function that, when applied to the net input of a neuron, determines the output of that neuron. The activation function almost always has an unlimited input domain, although by using a suitable function, usually a sigmoid function, the output range of the activation function can be limited. It is possible to choose any non-linear function, although for regression problems sigmoid functions are most commonly used. In this work the hyperbolic tangent, \( f_l(h_l) = \tanh(h_l) \), which has been shown to give a good performance in neural network models, is used as the transfer function for the hidden units. The \( \tanh \) activation function is a common function used in neural network modelling, having a function limit between \(-1\) and \(+1\) plotted in Figure 4.2. On the output unit there is no non-linear transfer
function and the contributions from hidden \( f_i \) and input layer \( i_k \) are only weighted \( \omega^{(h)}_{l,j} \) and \( \omega^{(h)}_{k,j} \), and a bias \( b_f \).

\[
f(x) = \tanh(x)
\]

**Figure 4.2** – Graph showing the \( \tanh(x) \) function, applied as the activation function in the neural network software, at each network node, developed by R. M. Neal

### 4.3.5 Bayesian Neural Networks

For decades there have been attempts to create computer programs and machines that can learn like people. The motivations for these developments being very diverse, being dependent on the background of the workers in the field of neural networks, examples of which can be found in the works of Rumelhart et al\(^{54} \), Hertz et al\(^{55} \), Bishop\(^{56} \) and Ripley\(^{57} \). To utilise a network properly and efficiently, certain methods need to be developed which will enable the weights to be adjusted in order for a node to produce an output or input to an adjacent node. A major problem that arises from the lack of knowledge on how the neurons in the brain receive information that enables them to apply the weights, thus any method of learning is unsubstantiated; development only being gained through results. The actual process of altering the weights to retain or learn an input pattern is referred to as a learning algorithm. For example, how do you teach a child to recognise what a chair is? You show him examples telling him "This is a chair; that one is not a chair" until the child learns the concept of what a chair is. In this stage, the child can look at the examples shown to it and answer correctly to the question "Is this object a chair?" Furthermore,
if the child is shown new objects, that it had not seen before, it is expected the child can recognise correctly whether the new object is a chair or not, providing that we've given him enough positive and negative examples. This is exactly the idea behind the 'Perceptron'.

The methods behind Bayesian learning follow a statistical route, using probability to express all forms of uncertainty. Simple application of the rules of probability can in theory be used to perform learning and other forms of inference. The results of Bayesian learning is a probability distribution over model parameters that expresses out beliefs regarding how likely the different parameter values are. Mackay introduced the use of Bayesian statistics to neural networks, successfully facilitating the training process. How a neural network model learns can be defined into two distinct groups depending on the techniques used; these are supervised, as used in the work described in this thesis, and unsupervised.

Supervised learning is a process of training a neural network by giving it examples of the task it is to learn. The way this is done is by providing a set of data pairs or vectors (patterns), containing an example of an input pattern that the network might have to process and an output pattern that the network should produce for that input known as a target output pattern. This technique is mostly applied to the feed forward type of neural networks.

Unsupervised learning is a process whereby the network is able to discover statistical regularities in its input space and automatically develops different modes of behaviour to represent different classes of inputs. Kohonen's self-organising (topographic) map neural networks use this type of learning. It is worth bearing in mind that the learning process of neural networks is about changing the state of connection between layers. Some algorithms involve changing the weights of the connections. However, other ones involve adding and removing connections as well as changing their weight values.

To start the Bayesian learning process, a prior distribution must be defined across the parameters, $P(\theta)$, that expresses the initial belief about the values of these parameters before any data are input. This step is considered a setback of Bayesian learning as it is not well understood how prior knowledge of the parameters affects the final model and this choice of a prior distribution is generally considered arbitrary. The priors are just a probability distribution on a particular region.
of the weight space, i.e. Gaussian distribution for the network parameters and Gamma distributions for the hyperparameters.

Given new data the network applies Bayes' rule to update the prior distribution, $P(\theta)$, to a posterior distribution, $P(\theta, y | \tilde{t}^{(t)}, \tilde{t}^{(n)}), \ldots, (\tilde{t}^{(n)}, t^{(n)})$, also the probability of network weights that fit the data well will increase.

$$P(\theta, y | \tilde{t}^{(t)}, \tilde{t}^{(n)}), \ldots, (\tilde{t}^{(n)}, t^{(n)}) \propto P(y)P(\theta | y) \prod_{c=1}^{n} P(t^{(c)} | \tilde{t}^{(c)}, \theta, y) \quad 4.2$$

$P(A | B)$ is read as the probability of B given A, where $P(t^{(c)} | \tilde{t}^{(c)}, \theta, y)$ is the conditional distribution or probability densities for the target and $P(\theta | y)$ is the prior density for the parameters. The $\prod$ symbol denotes multiplying a variable together across the given range (as $\Sigma$ does for addition).
Input Layer  | Hidden Layer | Output Layer
---|---|---

\( o = b^{(o)} + \sum_k \omega_k^{(io)} i_k + \sum_l \omega_l^{(ho)} f_l \)

\( f_l = \tanh(h_l) \)

\( h_l = b_l^{(ih)} + \sum_k \omega_{k,l}^{(ih)} i_k \)

**Figure 4.3** – Neural network architecture for a fully connected neural network containing 2 inputs, a single layer of hidden units containing 4 nodes and a single output.
The result of training a neural network through Bayesian methods is a posterior distribution over the network weights. Predictions based on previously unseen inputs give rise to a new distribution over the outputs stemming from the new data applied to the posterior distribution over the network weights, this output being a predictive distribution for the new data. The predictive distribution for a new output value \( t^{(n+1)} \), given the input \( \tilde{t}^{(n+1)} \) and training data \((\tilde{t}^{(1)}, t^{(1)}), \ldots, (\tilde{t}^{(n)}, t^{(n)})\), is given by:

\[
P(t^{(n+1)} | \tilde{t}^{(n+1)}, (\tilde{t}^{(1)}, t^{(1)}), \ldots, (\tilde{t}^{(n)}, t^{(n)})) = \int P(t^{(n+1)} | \tilde{t}^{(n+1)}, \theta, \gamma) P(\theta, \gamma | (\tilde{t}^{(1)}, t^{(1)}), \ldots, (\tilde{t}^{(n)}, t^{(n)})) d\theta d\gamma
\]

If a single-valued prediction is required, for example in a regression model, the prediction that minimises the expected squared-error loss is the mean of the predictive distribution, \( \hat{t}^{(n+1)} \). This optimal prediction is given by:

\[
\hat{t}^{(n+1)} = \int \alpha(\tilde{t}^{(n+1)}, \theta) P(\theta, \gamma | (\tilde{t}^{(1)}, t^{(1)}), \ldots, (\tilde{t}^{(n)}, t^{(n)})) d\theta d\gamma
\]

where \( \alpha(\tilde{t}^{(n+1)}, \theta) \), is the output of the network defined in equation 4.1.

### 4.3.6 Markov chain Monte Carlo methods

Evaluating equations 4.3 and 4.4 is a very complex process, mainly due to the complexity of the posterior distributions because of the large quantity of variables involved. This can be a major setback with Bayesian learning, though there are two methods typically used based on different approaches that can simplify the posterior distribution to make integration of the equations easier. The two methods are the evidence framework developed by Mackay\(^{58, 59}\) and the Markov chain Monte Carlo method developed by Neal\(^{53}\). The evidence framework is based on the optimisation of the hyperparameters and the approximation of the previous integral by a Gaussian centred on the maximum for the posterior distribution and single-valued estimates for the hyperparameters. Further information about this method, and C code used to apply the Mackay framework can be found at Mackay’s website\(^{60}\).
Problems have been seen to arise with the Mackay framework where Gaussian assumptions are inaccurate. A more accurate method, although still an approximation, is based upon sampling from the posterior, such as the Markov chain Monte Carlo method developed by Neal. This method is applied in the neural network software used throughout the work contained in this thesis.

The idea behind the sampling method is to approximate the integral in equation 4.3 over a sum as described below, equation 4.5:

\[
P(t(n+1) \mid T(n+1), (T(1), t(1)), \ldots, (T(n), t(n))) = \int P(t(n+1) \mid T(n+1), \theta, \gamma) P(\theta, \gamma \mid (T(1), t(1)), \ldots, (T(n), t(n))) d\theta d\gamma
\]

where \( t \) represents samples drawn from the posterior \( P(\theta, \gamma \mid (T(1), t(1)), \ldots, (T(n), t(n))) \). Such a series of samples may be generated using a Markov chain with the posterior as its stationary distribution. To estimate a single-valued prediction with respect to the posterior distribution, the Markov chain must have a unique equilibrium distribution, i.e. the posterior, which converges as rapidly as possible leaving the posterior distribution invariant.

In Neal’s work, a Markov chain that explores the entire posterior distribution is obtained by alternating Gibbs sampling, known as the ‘heatbath’ method, updates for the hyperparameters, \( \gamma \), with hybrid Monte Carlo updates for the network parameters, \( \theta \). This helps to explore weight space efficiently. An example of Monte Carlo implementation of Bayesian learning on neural networks is explained in detail by Neal and Rasmussen.

4.4 Strategies for Neural Network Computation

4.4.1 Data Pre-processing

Neural network analysis is usually carried out using variables that have been normalised; this normalisation is not essential to the neural network approach but allows a convenient comparison of the influence of individual input variables on an output. Several approaches to this scaling
process have been proposed in the literature, and can be found throughout the area of statistics. The linear scaling technique used in Mackay's\textsuperscript{63,64} model is:

\[ x_N = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} - 0.5 \]  \hspace{1cm} (4.6)

where \(x_N\) is the normalised value of \(x\) and \(x_{\text{min}}\) and \(x_{\text{max}}\) are the minimum and maximum values of \(x\) respectively from the entire data set.

This scaling is straightforward for all quantitative data, but for symbolic data 'yes' or 'no' values of +0.5 or -0.5 are used, as in binary 1 and 0. This technique is also used in the neural network modelling of weld metal properties carried out by Yurioka et al\textsuperscript{65}. Neal's\textsuperscript{53} neural network techniques used a normalising process that scales values such that they gain a zero mean. The technique used by Neal is known as linear normalisation and carried out as follows:

\[ x_{i,\text{norm}} = \frac{x_i - \bar{x}}{\text{std}} \cdot nstd \]  \hspace{1cm} (4.7)

where \(x_{i,\text{norm}}\) is the normalised value of \(x\), \(x_i\) is the actual value of \(x\), \(\bar{x}\) is the mean value of \(x\), \(\text{std}\) is the standard deviation and \(nstd\) is the new value of the standard deviation normally taken as 1.

Both techniques have been used throughout this work, with other methods also being found throughout statistical literature, the specific scaling being determined by the data type and activation function of the given neural network model. In this work the data is normalised around the zero mid-point of the \(\tanh(x)\) activation function of the neural network software. It should be noted that the gradient of this function at its extremes approaches zero, which can present a problem if the target value is at the maximum or minimum (-1 or 1). A potential method for this would be to alter the limits of scaling to avoid the ends of the activation function, as done with the linear scaling technique between -0.5 and 0.5. This works well with regression type problems, although for classification problems the output is not able to sum to 1 and therefore fails. A second problem is that the network is able to produce an output beyond the range of the input, for example 0.55, although in effect due to the stretching effect of outliers in the input data the full range of the activation function may not be used. Scaling of the data between -0.5 and 0.5 has an added advantage in that all data being considered has a maximum and minimum of equal magnitude, although this method requires good cleaning of the data to prevent unbalanced
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scaling caused by outliers. Normalisation on the other hand eliminates this to some extent by considering the standard deviation, however this does not cap the maximum and minimum of the data being considered.

Following scaling of the data, it is necessary to randomise all values before splitting into training and testing data sets to ensure that the training and testing processes covers all areas of the data domain represented within the specific dataset.

4.4.2 Training and Testing

The two important phases during the development of a neural network model are training and testing. Initially, the network architecture is chosen and the system is trained using a randomly chosen set of data examples. Vectors from a training set are presented to the network one after another. This results in the calculation, optimisation and application of the connection weights. If the network's output is correct, no change is made, otherwise, the weights and biases are updated using the Perceptron learning rule. Training is said to be complete when an entire pass of the training set has occurred without error. The next step involves assessment by inspection of the trained network, to determine the performance using unseen data.

A typical example of a run using Neal's neural network software, for a regression type problem, can be found in Table 4.1

The first command 'net-spec' creates a log-file containing the specifications for the network architecture and the priors to be used for the network parameters. Once the network has been specified, the network is used to model the targets. 'model-spec' specifies how the outputs will be used in modelling; in this example values are real-valued and modelled as the network output plus a Gaussian noise. The command line 'data-spec' specifies the file-name of the training and testing data sets, including the range of data to be considered within the file. The initialising phases are found in the command lines 'net-gen', 'mc-spec' and 'net-mc'. This initialisation phase is short, during which the hyperparameters and parameters take on moderate values, thus starting out the model with a degree of stability. The final two stages, 'mc-spec' and 'net-mc' are the major part of the modelling. The command line 'mc-spec' appends a new set of Markov chain
operations to the log-file. These operations are the Gibbs samples for both hyperparameters and parameters. The iterations of the sampling phase are started by the final command ‘net-me’.

# Commands to apply a Bayesian neural network to the simple regression problem.

net-spec example1-4h-log.net 2 4 1 / - 0.05:0.5:1 0.1:0.5 - x0.1:0.5 0.05:0.5:1 1
model-spec example1-4h-log.net real 0.05:0.5

data-spec example1-4h-log.net 2 1 / example1.DAT@1:125 . example1.DAT@126:250 .

net-gen example1-4h-log.net fix 0.5
mc-spec example1-4h-log.net repeat 10 sample-noise heatbath hybrid 100:10 0.2
net-mc example1-4h-log.net 1

mc-spec example1-4h-log.net sample-sigmas heatbath hybrid 1000:10 0.4
net-mc example1-4h-log.net 1000

Table 4.1 – Example of command lines used in regression type modelling using the neural network software

The parameters have been divided in 5 groups: input-hidden weights, hidden biases, hidden-output weights, input-output weights and output biases. It is necessary to specify a prior distribution for each group and for the noise expected on the data. These are specified in the ‘net-spec’ command line, broken down as follows:

\[
\text{net-spec file-name-log.net } Ni \{Nh\} No / ti [ ih \ bh \ \{hh \ ih \ bh \ th\} ] \{ho\} io \ bo
\]

- \(Ni\) – Number of inputs
- \(Nh\) – Number of hidden units
- \(No\) – Number of outputs
- \(ti\) – prior for the offsets of input units
- \(th\) – prior for the input hidden weights
- \(hh\) – prior for the hidden-hidden weights
- \(bh\) – prior for the hidden biases
- \(th\) – prior for the hidden unit offsets
- \(ho\) – prior for weights from a hidden layer to the outputs
- \(io\) – prior for input-output weights
- \(bo\) – prior for output biases

Following a ‘/’ the priors for groups of weights, biases and offsets are specified. If ‘-’ is specified instead of a prior or as in the case of ‘ho’ is omitted entirely; then the parameter in question does not exist, equivalent to them being equal to zero. The parameters captured between ‘{’ and means that they can either included or excluded.
Following trial and error experiments on the software, it is concluded that the choice of these priors is not crucial to the success of modelling, provided extreme values are not chosen. The training process will be able to infer the required parameters from the data. Noise parameters are gained from a Gaussian distribution with variance $\sigma^2$ or precision $\tau = \sigma^{-2}$. A so-called 'vague' gamma probability is then given to the precision allowing it to vary over a wide range. This gamma probability is given by:

$$p(\tau) \propto \tau^{\alpha-1} \exp(-\tau\alpha / 2\mu) \quad 4.8$$

and the values selected are $\sigma = 0.05$ and $\alpha = 0.5$, where $\alpha$ is the shape parameter, being specified in the 'model-spec' command line.

The input-hidden weights are given a three-layer prior; this is one more parameter than that used to describe the noise. Each weight is given a zero-mean Gaussian distribution of variance $\sigma^2$, this variance being controlled by the gamma distribution shown in equation 4.8. In the example the parameters used are $\sigma = 0.05$, $\alpha_0 = 0.5$ and $\alpha_1 = 1$. The same prior is given to the input-output weights. The hidden-output prior is given a two layer parameter, $\alpha = 0.1$ and $\sigma = 0.1$, the variance scaling according to the number of hidden units, details of which can be found in Neal's work$^{3}$. Output biases are given zero-mean Gaussian priors with a standard deviation $\sigma = 1$. The hidden biases group is given a prior consisting of two hierarchical layer, defined by a gamma distribution with $\sigma = 0.1$ and $\alpha_0 = 0.5$.

Network training begins with a short initial phase where the hyperparameters are kept constant at 0.5, allowing the weights to grow during 100 leapfrogs (finite time steps described in more detail in Neal's work$^{3}$). The short initial phase is followed by a long sampling phase, then the simulation is brought to equilibrium and a sample of 100 networks is produced from the posterior for use in prediction after Monte Carlo updates of 1000 leapfrogs.

Knowing when a Monte Carlo chain has reached equilibrium is generally a difficult task, for example, when the associated algorithm reaches regions of high posterior probability. A good
simulation is brought to equilibrium and a sample of 100 networks is produced from the posterior for use in prediction after Monte Carlo updates of 1000 leapfrogs.

Knowing when a Monte Carlo chain has reached equilibrium is generally a difficult task, for example, when the associated algorithm reaches regions of high posterior probability. A good way of approximating when the chain has reached equilibrium is by plotting the training and test sum squared error.

![Figure 4.4](image)

**Figure 4.4** – Example of errors in training and testing phases of neural network development for a network trained using 100 steps

In Figure 4.4 we see typical examples of training and test error behaviour for modelling simulations during the sample phase. In the example the initial 30 nets can be discarded and the remaining 70 networks (these are 70 different sets of weights), can be used to make predictions. This explained means that a single valued prediction will be the mean of the 70 guesses with the error as the standard deviation error.
This can be displayed as error bar values obtainable from the predictions of the neural networks from the Monte Carlo chain:

\[ sd = \sqrt{\frac{\sum(t-o)^2}{N-1}} \]  

where \( o \) is the mean value predicted, \( t \) is the 'real' value from the database and \( N \) the number of predictions, in this example 70.

### 4.4.3 Evaluation of Neural Network Model Performance

A potential problem with the use of powerful non-linear regression methods is the possibility of over-fitting the data. To avoid this problem, the data observations can be divided into two sets, a training data set and a test data set. The model is developed using the training data set. The idea of using a test data set is to then evaluate the behaviour of the model when presented with previously unseen data.

Figure's 4.5 and 4.6 show a model where data observations (\( y \)) should vary with a parameter (\( x^3 \)). The graphs represent the following:

i. Figure 4.5 (a) - Linear model – too simple, therefore it doesn’t capture the true complexity of data observed.

ii. Figure 4.5 (b) - Over complex model – accurately models the training data but generalises badly.

iii. Figure 4.6 - Optimum model, the model is at an optimum and fits the data well.

iv. Figure 4.7 - Training and test errors presented with reference to increasing model complexity.
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**Figure 4.5** - Predicted data points for a given data space fitting badly showing examples of (a) Linear model (b) Overfitting model

**Figure 4.6** - Predictions made for a given input data space, showing a model that generalises well

**Figure 4.7** - Training and test errors for increased complexity of a neural network model, highlighting the limit of test error given a continuous decrease in training error

Input parameters are assumed in the analysis to be precise and it is normal to calculate an overall error by comparing predicted values ($p_i$) of output against the measured values ($m_i$):

$$E \propto \Sigma_i (m_i - p_i)^2$$  \hspace{1cm} \text{4.10}$$

$E$ is expected to increase if important input variables have been excluded from the analysis. Mackay developed a useful treatment of neural networks in a Bayesian framework, which allows the calculation of error bars representing the uncertainty in the fitting parameters. This works by
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calculating a probability distribution of sets of weights to define fitting uncertainty, instead of calculating a unique set of weights\(^5\).

4.4.4 Input Relevance

To develop an effective neural network model, a number of parameters must be carefully controlled, including:

- Selection of an appropriate number of hidden units
- Normalisation of input and output data sets
- Initialisation of the weight factor distribution
- Setting of the learning rate and momentum coefficient
- Selection of an appropriate transfer function
- Generation of a network learning curve

Another important factor in any modelling is the use of the correct data; we assume that data inputs are true but, as Klein and Rossin\(^6\) suggest not all data collected are free of errors. These errors can have detrimental effects on the results gained from any modelling technique. In their work they compare linear regression models with neural network techniques, emphasising that a neural network is only as good as the training it has received. Therefore, data for training of a neural network must be as free of errors as is feasibly possible and a number of techniques for improving data quality and data evaluation methods have been explored.

A great variety of methods have been proposed to quantify the importance of inputs. The main conclusion is that there is no single measure of importance that is appropriate for all applications. In a linear model, i.e. a neural network without hidden units, each weight is the change in the output associated with a unit change in the corresponding input assuming all other inputs are held fixed. However, this interpretation depends on whether a single input can change independently of the other inputs. If the inputs include characteristics that one external operator cannot control and that are not independent, the interpretation has no base. Comparing weights in a neural network is more problematic than comparing weights in linear models, because now the simple interpretation does not exist due to the presence of the hidden layer.
Due to the weighted connections between nodes, if an input is irrelevant, the hyperparameter grows and forces the associated weights to vanish. A hyperparameter is the joint prior distribution of a common parameter’s components. For this method it is necessary to re-scale the inputs so that a one-unit change has similar significance for each of them. This idea is called automatic relevance determination, ARD, and it was introduced by Mackay and Neal. Then, by comparing the sigma’s, which control the weights outwards in each input, it is possible to get an idea of the important inputs. However, it is still not clear how good this measure is and how to interpret it in an architecture with input-hidden and input-output connections.

4.5 Other computational methods

Neural networks in their simplest form can be thought of as multiple regression techniques; multiple regression techniques being widely used throughout metallurgical and welding research to varying levels of success. The problem with using such techniques is that highly complex relationships are fitted too simply, and therefore generalisation of such models can be poor. In an effort to model more complex data relationships, considering regression, classification and real time situations various techniques have emerged, using probability theories, evolutionary techniques and cognitive methods.

4.5.1 Fuzzy Processes

Data inputs to a neural network are not always hard physical values; these data may include subjective responses, or badly defined categories. Similarly output from the network may not be a precise number. Therefore, increased measurements of these subjective or imprecise data may be required, which can lead to overwhelming amounts of data for the neural network. Fuzzy set operations are grounded on a solid theoretical foundation, dealing with imprecise quantities in a precise well-defined way. For example, the statement, “today is sunny”, might be 100% true if there are no clouds, 80% true if there are a few clouds, 50% true if it’s hazy and 0% true if it rains all day. The rules set in place allow the fuzzy processor to determine the percentage membership to a category given the conditions.

One of the advantageous properties of fuzzy set approaches is that contradictions in data need not cause problems. Conventional rule-based methods require special arbitration procedures, with data fitting into distinct groups with no overlap. Fuzzy processors manage to distinguish
data points lying on the borders of these groups, and identify how much they belong to each group.

In fuzzy set theory observations can partially belong to pre-defined sets, in contrast to traditional Boolean logic, in which membership is an all or nothing proposition, see for example Figure 4.8 and 4.9. The membership functions define whether a data point has full or partial membership of a group. The rules that govern this can make or break a fuzzy processor; these are further examined by Masters.

Figure 4.8 – Schematic representation of Boolean logic membership – Boolean logic demands definite membership of a set
Fuzzy processes are used a great deal in the area of control and in-process evaluation of automated manufacture. Much work can be found in the literature as to research conducted on the application of fuzzy neural networks into automated weld processes. Gao et al\cite{69}, incorporated both neural network techniques and fuzzy processes in control of a mechanised gas tungsten arc welding machine (GTAW). By using a visual sensor, they utilised a neural network to estimate penetration depths based on weld parameters, and the image of the molten pool. Rashid et al\cite{70}, considered the use of fuzzy logic controllers in seam tracking for pulsed gas metal arc welding, by utilising the average voltage signal as a control signal for the fuzzy logic controller, in weld seam tracking of v-welds.

4.5.2 Gaussian Processes

Gaussian processes have a statistical nature needing only a small representation of data from a problem, and in the Gaussian approach the distribution of data is directly defined. The Gaussian process model assumes that the joint probability distribution of any N output values is a multivariate Gaussian. In Bayesian neural networks, this joint distribution is a complex function involving integration over all possible settings of the parameters weighted by their prior probability distribution.

Mackay et al\cite{71} compared the use of neural networks with Gaussian processes in the modelling of the yield strength of nickel-based super alloys. The comparison was with a committee of 5 artificial neural networks individually trained and optimised on one half of the data and tested on
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the other half. The work concluded that a committee of neural networks and Gaussian process methods are able to predict with similar confidence well-known metallurgical trends. Importantly, however where data were missing or widely separated, both models showed a low level of confidence. An advantage of Gaussian process models is that the labour intensive process of selecting optimum models, using test set evaluation is not necessary. However, Gaussian process models are computationally time consuming, with computer time increasing with the size of the database cubed, whereas in the case of artificial neural networks the computer time is independent of database size. Therefore, it was concluded that Gaussian process models would be preferred for handling relatively small data-sets due to ease of use, and artificial neural networks would be preferred where data-sets are comparatively large, for efficiency in computing.

Neal uses Gaussian processes to define prior distributions over input variable sets, using this technique in both regression and neural network techniques\cite{53,72}. This technique is also used in earlier work by Mackay\cite{59}, where he gave the network weights and biases Gaussian prior distributions, helping to eliminate the problem of uncertainty in initial values.

4.5.3 Genetic Algorithms

A genetic algorithm works by natural evolution, yielding the global optimum solution to a problem, without any specific prior knowledge about the problem to be solved. However, for a genetic algorithm to be applicable, potential solutions to a given problem must be presented as strings of numbers (usually binary) known as ‘chromosomes’. The genetic algorithm then creates a population of solutions and applies genetic operators such as ‘mutation’ and ‘crossover’ to evolve the solutions in order to find the best ones. Initial populations of ‘chromosomes’ are usually created using a random number. Further detail and discussion of genetic algorithms can be found in the paper by Pham and Pham\cite{73}.

Genetic algorithms have found applications in engineering problems involving complex combinatorial or multi-parameter optimisations. Some examples are configuring transmission systems, generating hardware description language programs for high-level specification of the function of programmable logic devices, designing the knowledge base of fuzzy logic controllers, planning collision-free paths for mobile and redundant robots, and scheduling operations of a job shop.
4.6 Application of Neural Networks

Neural networks and other forms of artificial intelligence have seen a rapid increase in their inclusion in engineering and real world applications. Pham and Pham outline the five major types of artificial intelligence seen in engineering applications: knowledge based systems, fuzzy logic, inductive learning, neural networks, and genetic algorithms.

In 1992 the 'advisory council on science and technology' put together a report outlining the issues relevant to exploitation of neural computing and the benefits to British industry. The report to the government concluded that neural computing was at a significant maturity, with a small but enthusiastic research base in the UK, with some R&D in larger technologically oriented companies. It was outlined that there is a high superficial awareness for an emerging technology, although the radical and persuasive nature of its potential could present a significant hurdle to its adoption. In reply the government acknowledged the proposals, and a need for increased awareness throughout industry.

4.6.1 Application of Neural Network Modelling to Physical Metallurgy

The development and processing of materials is complex and quantitative evaluation of many phenomena is difficult to achieve. The lack of progress in predicting mechanical properties of materials can be related to their dependence on large numbers of variables. It is, however, possible to identify clear patterns, for example the toughness of a steel can be improved by making its microstructure more chaotic so propagating cracks are more easily deflected, and therefore qualitative relationships can be established based around experimental data. Neural network models become extremely useful in such cases, not just in the study of mechanical properties, but wherever a complex problem becomes overwhelming from a fundamental perspective, and where simplification of the model would be undesirable.

Bhadeshia has reviewed the use of neural networks in the material sciences field, comparing linear regression with the non-linear capabilities of neural network modelling. The comparison is with a model developed by Mackay incorporating a Bayesian framework from which the neural network is based. In particular, the use of neural networks in modelling weld metal
toughness, the tensile strength of steel welds, weld cooling rates and hot cracking of welds were discussed. Additionally, the applications of neural networks to wider metallurgical issues, such as the prediction of the strength of Ni-based super-alloys and methods of microstructure prediction have been reviewed.

4.6.2 Application of Neural Networks to the Welding Process

Welding processes have seen major applications of neural network models. An example is in weld seam tracking where a trained neural network is used to control a welding robot by interpreting the output from sensors. Suga, Yasu et al\textsuperscript{8} have developed a new control system for a seam-welding robot which involved inputting a binary image into the neural network to enable recognition of weld line direction and tracking. Neural network techniques have also been studied by Rock et al\textsuperscript{9} in the real-time visual tracking of seam welds. In order to accurately track the seam weld with a robot arm accurate high-speed image analysis is required from the camera inputs. The use of a neural network allows fast processing of camera positioning, arm relative positioning and elimination of noise from weld splatter and weld seam surroundings.

Yamane et al\textsuperscript{10} considered the problem of weld pool depth control in robotic welding. In-process measurement of weld pool depth is difficult during operation, and therefore a neural network was used to estimate the depth from welding parameters including weld pool-shape, groove gap and welding current. The output from the neural network was then used as an input to a fuzzy controller to improve weld quality in real time operation. Suga et al\textsuperscript{8} have also developed neural network techniques for penetration control in TIG (Tungsten Inert Gas) welding by measurement of the molten pool shape. By using visual sensors on an intelligent welding robot system, welding conditions can be controlled by means of feedback from neural network processing. Matsuyama\textsuperscript{12} develops his ideas for nugget size sensing for spot welding based on neural network learning. The system is being developed for use in quality control, without the need for destructive testing techniques. The neural network considers a dynamic voltage between welding tips and weld current waveforms as the monitoring parameters for nugget size.

Optimisation of welding processes is a key factor in quality control. Tay and Butler\textsuperscript{13} presented a case study on the optimisation of a MIG (metal inert gas) welding process. By integrating experimental designs and neural network technologies, they considered optimisation of the MIG
welding process of medium carbon steel tubular drilling products. Their first objective was to look at improving weld quality, maximising penetration whilst minimising bead width and height, and secondly they required predictive learning and modelling capabilities of the weld quality characteristics. Training data were collected from experimental design methods and input to a GaRBF (Gaussian Radial Basis Function) neural network, which was used to optimise the basic welding parameters. The neural network architecture and input parameters can be seen in Figure 4.11. In this neural network fine-tuning capabilities were built in, and additional data could be used at any time for further refinement of the model. This refinement could be used where it may be more economical to use a training data set that does not quite fit the situation exactly, thereby being refined by a small secondary training set. Two papers by Gunaraj and Murugan consider the optimisation of weld bead volume in the SAW process, proposing mathematical models to predict and optimise the welding process.
Zeng et al developed neural network techniques to optimise both manual and automatic TIG welding. Using the back-propagation network derived from the Rummelhart model, two neural network models were devised. The first model was developed to optimise parameters of the manual TIG welding process. Manual TIG welding is a two-handed process, and close control of torch and filler angles, welding speed, filler rod feed technique, arc length, gas shielding and back purging are required for good quality welding. The neural network developed used a combination of numeric and symbolic inputs; a symbolic input taking the form of a 'yes' or 'no' (1 or 0) binary form. A nine input model was constructed with six symbolic inputs; mild steel, stainless steel, flat position, H/V position, vertical position and overhead position, and three numerical inputs; sheet thickness, joint gap and filler rod diameter. Five numerical outputs were mapped to these inputs; current, voltage, filler rod consumed per metre of weld, weight of weld metal per metre of weld and arc time per metre of weld. The network was trained using 40 input/output data pairs, eight for mild steel and 32 for stainless steel, with eight data pairs for each position, using commercial neural network software. From the results a two layer neural network was constructed with an error tolerance of 0.04, which predicted all welding requirements within this tolerance.
The second neural network model considered the more complex problem of welding parameter inspection in mechanised tungsten inert gas (TIG) welding. Mechanisation of the process increases speed, and uniformity of the welded structure, but for weld quality to be maintained, greater attention must be made to accuracy of joint fit-up and welding parameters. A different approach was taken this time, and a combination of two separate neural networks was created, each considering welding with and without filler respectively. Numerical inputs taken from in-process monitoring were used; plate thickness, weld current, weld voltage, welder travel speed and filler wire feed rate. Both sub-networks consisted of two hidden layers, outputting symbolic values as a control feedback. The network was trained with 77 input/output pairs for welds without filler, and 88 input/output pairs for welds with filler. The results concluded that all predictions were within the set tolerance.

Use of artificial intelligence (AI)-methods, such as neural networks, to simplify and improve parameter optimisation and quality of Gas Metal Arc (GMA) welds was investigated by Dilthey and Heidrich. Consideration of weld parameters, through a combination of neural network and genetic programming techniques enabled development of optimal weld parameters. Several software packages were incorporated in this study in the processing and development of neural network models. Commercial neural network software was used, with the finished network being exported into the C programming language allowing ease of integration into quality monitoring systems. In addition to the neural network simulation software, three additional pieces of software were developed to compliment the commercial software. Three pieces of software were developed allowing preparation of network training and analysis of the results of the training phase, calculation of seam quality using the data of a laser scanner, optimisation of the trained networks based on different criteria, using methods of genetic programming. The software was then used to find suitable optima for the welding process, this optimum being ‘high welding quality with high welding speed’.

4.6.3 Prediction of Weld Metal Chemistry and Microstructure

Little information has been found in the literature on the use of neural network techniques for modelling of weld metal chemistry and microstructure. The majority of modelling undertaken on weld metal chemistry in the literature has been undertaken for given sets of parameters or a specific weld manufacture process, and therefore a relatively simple relationship exists between
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weld chemistry and chemistry of parent plate and consumables in these cases. Therefore, most weld chemistry modelling can be performed by simpler, cost effective, linear methods. Many physical models of the microstructure of weld metals are also found in the literature, for example Bhadeshia and Svennson. Physical models provide a better understanding of the problem, and therefore where these models exist neural network modelling is unnecessary.

Regression analysis is a statistical method that utilises the relation between two or more quantitative variables so that one variable can be predicted from the others. This is in contrast to neural networks that are non-linear, and utilise complex relations in the data, though they are similar in their application. The term linear does not refer to the shape of the resulting curve (i.e. a straight line), but to the fact that in the functional representation;

\[ F(x) = p_1 \cdot f_1(x) + p_2 \cdot f_2(x) + p_3 \cdot f_3(x) + \ldots \] 4.11

the coefficients \( \{p_i\} \) appear only to the first power (i.e. in linear form). In this case, the overall function \( \{f(x)\} \) is expressed as a linear combination of a set of functions \( \{f_i(x)\} \), which are known as the basis functions for the regression.

This methodology is used widely throughout business, the social and behavioural sciences and engineering fields. Many examples of this technique being applied to materials science, and in particular welding, can be seen throughout the literature. Thewlis and Dainty developed multiple regression models for the chemistry of submerged-arc seam welds, considering the chemistry as a mass balance equation. A more fundamental approach to this can be found in the paper by Thier, where he considers dilution of parent plate and consumable.

Neural network techniques have been employed in the prediction of submerged-arc weld metal chemistry. The database used consisted of experimental 3-wire submerged-arc welds, manufactured under laboratory conditions using a single flux, with varying weld condition parameters. Use of a neural network with 5 inputs was found to improve on this, with increased inputs up to 7 not giving any appreciable improvement in prediction, as shown in Figure 4.12.
Figure 4.11 - Average sum squared error on test data predicting weld composition of each element in the database using different models taken from Perez-Perez et al\textsuperscript{90}

Vitek\textsuperscript{91} developed a neural network method for predicting the ferrite number in austenitic stainless steel welds. Ferrite number is an arbitrary value designating the ferrite content of an austenitic stainless steel weld metal. This value directly replaces the percentage ferrite or volume fraction ferrite, and can be determined by magnetic testing. Prediction of ferrite number can be key to determining the properties of a weldment, and is also a strong indicator of the tendency of austenitic steels to crack. In Vitek’s work he used a commercial package incorporating the back-propagation method. In the work two neural network models were developed, making use of the same data set of 961 points. Both networks used inputs of elemental concentration, with an output of ferrite number, although the second network used 5 more inputs than the first, which used 8 inputs. 90\% of the available data were used for training, with only 10\% used in testing of the neural network. This work showed that the use of neural networks was a considerable improvement over conventional means of predicting ferrite number, with limiting factors being the size training data set and consistency of data. This work is further discussed and developed in Vitek’s\textsuperscript{92, 93} later work describing the optimisation of the neural network for predicting ferrite number. The papers identify optimum architectures and network parameters, comparing accuracy of network models and the results obtained.
techniques, to predict the heat input and the area of the HAZ. The findings showed that the open circuit voltage and wire feed rate had a positive effect on the area of the HAZ, whilst welding speed and nozzle to plate distance have a negative effect on the area of the HAZ.

Solidification cracking can occur in welds during cooling from the liquidus temperature. When fluid flow or motion of solid components cannot accommodate density changes associated with solidification and thermal contraction, cracking occurs. Solidification cracking depends partly upon the chemical composition of the weld metal, due to the dependence on solidification temperature. Other dependent factors are the cooling rate and weld geometry. Ichikawa et al. have used neural network techniques to predict cracking in a weld by considering chemical composition and weld parameters. Mackay's techniques were used in the modelling, choosing input variables from knowledge of metallurgical concepts. A binary output was used for the network, where '1' represented 'cracked' and '0' represented 'no crack'. As data were collected from the literature, not all systems adopted this approach therefore where a crack was represented as a measurement or ratio; 'no crack' was representative of welds with a crack ratio less than 0.05. Training was undertaken with half the data, 432 models were obtained, by varying the number of hidden units, random seed and initial weights. The best 126 models were selected for examination to construct a committee of models. Exhaustive testing was carried out in order to ensure that the selected model predicts in a way consistent with metallurgical experience. The authors conclude that the model selected was successful in representing solidification cracking of low alloy steels. The model was seen to demonstrate reproduction of known metallurgical experience and plans to update the model when further data are available are suggested.

4.6.4 Prediction of Weld Metal Properties

Regression models used in the prediction of toughness require the use of many variables. However, this does not properly simulate the behaviour because the relationships between the parameters affecting weld toughness are non-linear. The yield and ultimate tensile strengths of steel welds were modelled using neural networks from published data in the work of Cool, Bhadeshia and Mackay. The work found that throughout the literature the common problem was incomplete data sets, which limits the functionality of the models. A common problem with data modelling is the collection of suitable input data; Lalam eloquently covers the issue of compromise between size of data set and the number of inputs to accurately model a problem.
The number of appropriate data pairs available diminishes as the number of input variables increases, and means that the number of variables used in the prediction of properties may have to be reduced. The work resulted in a model capable of estimating the strength as a function of chemical composition, welding conditions and heat treatment parameters. By the use of Bayesian methods, allowances for model uncertainty could be included, identifying areas requiring detailed investigation. The model was implemented in the prediction of power plant alloy properties, although it was noted that the model had much wider applicability because the data applied in training of the neural network came from all varieties of welding materials.

Lalam et al. also used neural networks as a means of non-linear regression analysis, using the neural network techniques proposed by Mackay. Lalam studied the Charpy impact transition temperature for ferritic steel welds, using the neural network as a means of inferring more meaning from the data. In particular, a comparison was made of errors from a single neural network compared with a committee of neural network models; the committee being far better due to the ability to select the best performance areas from several models. The use of a committee overcomes the problem of having to choose the complexity of a neural network architecture. However, it was found that neural networks did not reduce the levels of noise perceived in the measured values of transition temperature due to the high number of dependent variables compared with the small data set studied.

Yurioka et al. considered the analysis of tensile strength, FATT (fracture appearance transition temperature), and hardness of high-heat input SAW welds. The authors collected data from the literature, gaining a wide spread in the variation of the data also using the technique of Bhadeshia, Mackay et al. The work successfully managed to train a neural network model to predict tensile strength, FATT and hardness, though some specific points in the hardness predictions were found to show relatively large error bars. This was explained by the small number of data sets used in training the network for hardness predictions.

Two papers by Lalam et al. consider the estimation of common mechanical properties of ferritic steels using neural network techniques. In the first paper neural network techniques are used in the prediction of yield strength and UTS of ferritic steel welds. Using Mackay's methods neural network models were formed for ferritic welds, manufactured using the manual metal arc (MMA), submerged-arc (SAW), and tungsten inert gas (TIG) processes. All data were
collected from published literature, therefore the welding process was only represented by a global heat input which enabled the formation of a data set without missing values. Over 80 neural network models were trained, using 50% of the data for training and 50% for testing the neural network models. Each model had 19 inputs with model variance being in the number of hidden units used or the random seed used in initiation of weights in connections. As is expected, the more complex the model the lower the perceived noise in training, although the testing found that three hidden units gave an optimum performance. Further to this a committee of models is considered, taking optimum properties from several models, these optimum properties being ranked using the log predictive errors. Log predictive error, unlike test error reduces the penalty for making a wild prediction, so long as large error bars accompany the prediction. Larger values of the log predictive error imply a sound model. The size of the committee is evaluated by considering the error against the size of the committee, the test error associated to the best single model was found to be clearly greater than that of any of the committees of models. Similar work has been carried out for UTS, using committees of neural network models. Trends were found to be consistent with what is expected metallurgically, though this paper covers only simple trends due to the large number of variables involved.

Lalam et al\textsuperscript{97} also discuss the mechanical properties of ferritic welds that are more difficult to model than those in the earlier work, considering the modelling of elongation and Charpy toughness. Their elongation model consisted of 20 inputs considered to influence the ductility of the material. The authors argue that certain other parameters could be suggested, but due to the restrictions in database construction for neural network purposes and inconsistency of data in the literature only some of the parameters would give rise to an adequate amount of data. As is common throughout the literature the amount of data obtainable diminishes with the increased number of parameters required from the data. Several neural network models were trained, with a variable number of hidden units and random seed generator used in initiating the weights. The models were then put into a committee and the comparison between committees and single models yielded the best model to be a committee of 58 models. For Charpy impact toughness a similar method was applied with two more inputs, defining the test temperature, and nitrogen concentration. The paper concludes that it is feasible to create reasonable neural network models for both tensile elongation and Charpy toughness, taking into account chemical composition and heat treatments and a number of weld parameters. The biggest problem defined by the authors,
and indeed generally true, was down to data availability, and the uniformity in distribution of data found.

4.6.5 Prediction of Physical Dimensions of a Weld

Prediction of weld profile shape as a function of weld process conditions is desirable in understanding what the influence of changes in these conditions have on the final weld profile. Lee et al\textsuperscript{100} discuss the parameter changes that influence the shape of the bay area in arc welds, and conclude that the major influencing factors are heat distribution from the arc, current density and electrode diameter. Lee et al\textsuperscript{100} also cover the effects of welding parameters on the size of heat affected zone in submerged-arc welding. Hirata et al\textsuperscript{101} consider the effects of chemical composition on bead formation in TIG arc welding and note that certain chemical additions affect surface tensions during the liquidus stage of the weld metal. Increases in S content were found to improve penetration, explained by the inducing effect on generation of inward convection in the molten pool. Mn also had a positive effect on penetration, the preferred explanation being the ability to increase current density in the anode region. S content was also the cause of deterioration of weld bead shape uniformity; the assumed explanation for this is the contraction of the anode area, thus any slight movement caused the molten pool to move and become unstable.

Vitek\textsuperscript{91} discusses the use of neural networks in the prediction of weld profile shape as a function of weld process conditions for pulsed laser aluminium welds. By using inputs of welding speed, average power, pulse energy, and pulse duration, a neural network was trained with the weld profile shape as the related output. A method is shown for identifying weld profile shape, by using weld area, depth, width and half width as output from the neural network, see Figure 4.18. A separate routine was used to match up the values to actual experimental weld profiles, thus enabling prediction of a final weld pool cross-section. Despite this work being carried out with only a small training data set the predictions were found to be good, and variations were within those found in the experimental welds.
Similar work has been carried out by Chan et al\textsuperscript{102}, who considered the use of neural network technology to predict gas metal arc (GMA) weld geometry. The models considered the bead shape as a function of bead width, bead height, penetration bay angle and bay length (the distance from the mid-point bead width to the bay region and the angle of this distance). They also considered the use of area as a reinforcing parameter. Modelling was carried out using a back-propagation network configuration. Dilthey et al\textsuperscript{103} also carried out a classification exercise using neural networks as a quality surveillance tool in online GMA (gas metal arc) welding. Similar to the problems discussed in this thesis, this type of welding has no analytical approach to modelling because the process has many complex phenomena to consider. Their work considered the various parameters controlling the process compared with the weld bead quality output in order to allow for online monitoring to highlight when the quality of a weld is considered substandard due to the process parameter measurements.

Weld quality is strongly characterised by weld pool geometry, which in turn plays an important role in determining mechanical properties of a weld as described by Sacks\textsuperscript{104}. Tarng et al\textsuperscript{105} use neural network modelling techniques to relate welding process parameters with features of the weld pool geometry for TIG welds without a filler and using a backpropagation network. The inputs, obtained from a series of experimental welds, were arc gap (2.4 – 3.2 mm), inert gas flow rate (5 – 10 l/min), welding current (80 – 100 A), welding speed (25 – 30 cm/min) and cleaning percentage (30 – 70 %), which were mapped to three output weld geometry features; front depth, back height and back width. The best network was found to contain two hidden layers, having a
5-8-6-3 configuration comprising of five inputs, eight nodes in the first hidden layer, six nodes in the second hidden layer and three outputs. The results showed that after training the average sum squared error of predictions was found to be less than 0.001. Zhang et al.\textsuperscript{106} used similar techniques for real-time measurement of weld pool geometry to determine weld pool characteristics in gas tungsten arc (GTA) welding. A commercial neural network software package was used, incorporating the extended delta-bar-delta (EDD) algorithm. This overcomes slow convergence associated with conventional back-propagation methods, as each connection weight has its own self-adapting coefficient. Inputs to the network were weld pool length and nine relative widths corresponding to outputs of polar co-ordinate model parameters. 8000 data sets were used in training the network, with a single hidden layer of twenty elements being found to give best convergence. For the real-time investigation the neural network is incorporated with an image sensor, image processor and welding machine, as outlined in Kovacevic et al.\textsuperscript{107}. Due to the use of real-time image processing and the neural network, parameters can be calculated in approximately 200 ms. The work found that the geometrical appearance of the weld pool can be characterised by the proposed co-ordinate model, and that by the use of neural networks and real-time processing of images specified characteristics can be determined mid-process. The weld penetration can also be found accurately by using full geometric information of the weld pool. The paper suggests that for further development of a practical control system, the number of parameters used should be minimised thus reducing computer time.

Identification of defects in weld metal by non-destructive testing (NDT) is an advantageous method of saving money while ensuring quality standards. Ultrasound inspection is a principal technique in detection of defects in metal structures. Although the detection of defects is the first objective, it is equally important to characterise the nature of the flaw. Baker and Windsor\textsuperscript{108} cover the application of the Hopfield neural network\textsuperscript{109} method to classify weld defect types using parameters extracted from ultrasonic measurements. The Hopfield method is the most straightforward of neural network techniques, storing information in a binary format, representable as a black and white image. The advantage of the Hopfield neural network technique is that it has a simple non-iterative learning procedure. Artificially manufactured defects were obtained each of a known type, creating a data set of 83 known defects. The raw data obtained from the ultrasonic testing took the form of time-of-flight scans as a function of position over the defect, taken at three differing angles of incidence. Parameters were represented as six different features of the ultrasonic pattern; waveform sharpness, amplitude variation, shape
of reflected signals, waveform duration, rms amplitude with angle, and deviation from best fitting plane. The Hopfield neural network algorithm was shown to be capable of classification of weld defect types using the feature parameters extracted from ultrasonic measurements. The performance was found to be comparable to that of conventional weighted minimum distance classifiers. It is highlighted, however, compared with more advanced neural network algorithms, such as back-propagation methods, confidence was poorer. Further work being considered by the authors appreciates the simplicity of the Hopfield technique and therefore makes use of a more advanced Rumelhart layer network. This technique repeatedly presents patterns from the training data to the network, with synapse weights adjusting accordingly so as to achieve lower error in output. The use of a backpropagation neural network technique is described by Aoki and Suga, using data from X-ray radiographic testing methods to determine weld defects, in a similar fashion to Baker and Windsor.

Dilthey and Dickersbach worked on a neural network technique designed for the quality evaluation, by non-destructive means, of resistance spot welds. Time dependent factors, such as voltage and current application were measured for input to the neural network. Steel and aluminium were considered in this study, both requiring different types of neural network modelling. As the aluminium went through more complex behaviour during welding, due to the added care required when welding aluminium compared with steel, more complex neural network architectures were required. The welds were manufactured using a set of 20 different manufacturing conditions, giving varied quality in the welds. These were then evaluated by means of a shear strength test. This information from the manufacture, and evaluation stage could then be fed into a neural network for training purposes. Once a satisfactory number of samples have been processed through the training stage, the application of the neural network to in process quality assessment could begin. This removed the need for destructive testing of spot welds. The work concluded that the neural network performed with relatively high confidence in the quality evaluation of both steel and aluminium welds. Similar work has been carried out by Cho and Rhee using dynamic resistance measurements as a form of input to the neural network.

The diameter of weld nugget in spot welding is a useful measure of the quality of the weld. Brown et al look at the conventional methods presently used in predicting the quality of welds manufactured by the resistance spot welding process, and look at the use of neural networks.
taking inputs based on the entire dynamic resistance curve for the process. Data used came from electrode life testing, using hot dip galvanised steel. The resistance-time relationship across the welding electrodes was calculated from the measured welding current and welding voltage. A 50kVA short throat spot-projection-welding machine was used for electrode heating. Carbon imprints were taken at intervals during testing to establish the electrode diameter wear, this information being required to take account of effects of electrode wear on the resistance waveforms. Data was pre-processed into a suitable input form for the neural network, with approximately two-thirds of the data being used for training. Supervised training, employing the standard back-propagation algorithm, was used to minimise the error between the measured and predicted weld diameter during training. Training was optimised by interrupting the training stage at given intervals to check that convergence was being maintained, thus eliminating over-fitting of the data. The work found that 70% of all predictions of weld diameter were within 0.5 mm (± 0.25 mm) and of those patterns considered to be incorrect, 18% predicted weld diameter within 1 mm (± 0.5 mm), giving an 88% success rate. Bad welds defined by a diameter less than 3 mm were successfully identified in approximately 90% of cases. A similar evaluation of Gas Tungsten Arc (GTA) weld pool characteristics modelling by neural network techniques is given by Karsai et al114. The paper compares the results of neural network techniques with more traditional methodologies, presenting the findings numerically.

Chang et al115 used neural networks to compare the prediction of laser spot weld shape with existing numerical methods. The numerical method considered was finite difference analysis, considering temperature, thermal conductivity, heat source generation, reflectivity, thermal diffusivity, absorption, beam radius and laser power. This model was simplified somewhat, with certain parameters being omitted. The work concluded that both models had their individual merits, and noted that by combining both models a more precise model can be achieved.

4.7 Accountability – Use of Neural Networks on Real World Data

In 'real world' applications neural networks must be proved to be accountable; it is not sufficient to produce output data from a network without any information as to the quality of that data. In many industrial applications there are considerable financial implications attached to the subsequent use of inaccurate, incorrect or misleading output data. Helliwell et al116 outline the need for reliability and confidence in neural networks, and the dangers of reliability on results
without information as to quality of that data. In “real world” applications it is rare to have training data that covers the entire input space. Hellwell defines the quality of neural network output in five key points:

- representative nature of the original training data in relation to the scope of the problem domain
- properties of the network
- whether the generalisation point lies within the domain of validity of the network
- density of training data within the region of the generalisation point
- quality of the training data within the region of the generalisation point.
4.8 Chapter Summary

From the literature it is clear that neural networks can play a vital role in modelling data from many different areas, including that of welding. With the improvement in speed of today's computers they are becoming more and more of a viable option, especially when compared with their roots back in the 1960's and 70's. Throughout the 1990's through to the present day neural networks have become more fashionable within the metallurgical fields, being incorporated into a variety of theoretical and manufacturing applications.

With the drive towards cost efficient manufacturing the desire to reduce the cost and time-scale of experimental trials and decrease the number of rejected products there is a need for alternative methods of determining the desired parameters for manufacture. This is especially important in the manufacture of line-pipe, where any experimental trials slow production and carry high overheads. From the literature is seen that many welding applications have utilised the flexible modelling ability of neural networks, applying them at a manufacturing level as on-line quality control and as predictive tools of various chemical, geometrical and mechanical properties for single wire, laser and spot welding processes. Very little literature has been found in which neural networks, or any other quantitive techniques have been applied to multiple wire systems as found in the submerged-arc welding of line-pipe. This is therefore the subject of the following chapters in which neural network techniques are developed to cover chemical, geometrical and mechanical property characteristics of multiple wire submerged-arc welds.
Chapter 5 - Neural network modelling of weld metal chemistry and microstructure

5.1 Introduction

The first step in applying a regression or neural network technique to a large database is to determine which variables are necessary as inputs. Through application of metallurgical knowledge, and by looking at previous regression and neural network models from the literature, the parameters to be considered were established. Previous work at Loughborough University\(^{90}\) has shown that modelling of weld metal chemistry and mechanical properties can be done, giving a good starting point for which parameters should be considered.

The first section of this chapter considers the modelling approach of Perez et al\(^ {90}\) and then models a revised version of the data used in their work for the prediction of weld metal chemistry from plate and wire chemistries. This work is further developed using more complex data arrays, showing that significant improvement in the neural network modelling of weld metal chemistry can be achieved.

Following on from the chemistry predictions, this chapter then discusses the modelling of the weld metal microstructure content, using chemical composition for the weld metal and process parameters governing the thermal cycle experienced during the welding procedure as inputs. The principle behind this is that chemistry predictions from the first models could be used in the modelling of weld metal microstructure. Successful modelling is achieved for the acicular ferrite content of the weld metal, this being found to be more accurate than modelling multiple microstructural constituents and justifiable metallurgically given that the largest fraction of the microstructure is expected to be acicular ferrite.

The final section of the chapter uses a limited data set in the prediction of the occurrence of hydrogen-induced cracking (HIC) in weld metals. This work is different in that it considers the use of a binary output model and indicates the presence of HIC cracks or not dependent upon the welding process parameters and weld metal chemistry. This work shows 95% accuracy within the constraints of the very limited dataset available.
5.2 Early work modelling weld metal chemistry using neural network techniques

From the work of Perez-Perez et al, the parameters found to be important in considering weld metal chemistry were as follows; plate thickness, heat input, wire stickout, concentration of element X in plate before welding and concentration of element X in wire consumable. Further parameters to consider with more complex or poorly fitted data would be; identification of inner or outer diameter weld position and identification of tack weld type, i.e. whether it is intermittent or continuous. These additional parameters do not have a specific numerical value, but have to be represented by a binary type system, using 1 or -1 to distinguish between the two variables, comparable to '1' and '0' in the binary system or 'on' and 'off'. Note this system is only considered where normalisation of data is carried out to a zero mean and standard deviation equal to 1.

5.2.1 Description of data used

From the modelling described in section 5.2, a desired output of the concentration of the element X in the weld metal can be predicted. The data provided are separated into three data sets for each prediction parameter being considered, classified as:

- Training
- Testing
- Validation Set

The majority of the data are used in the training and testing of the neural network model, however a small portion of data is held back for use in evaluating the predictive capability of the neural network model. The data examined came from the 3-wire experimental submerged arc weld database, produced at the Corus, Swindon Technology Centre in Rotherham. These welds were made under production conditions to gain knowledge of the effects occurring upon varying welding parameters. The flux used was the same throughout the welds and therefore flux was not used as an input parameter for the chemistry of the weld metal. The numbers of cleaned data used in the evaluation of each element considered are shown in Table 5.1. Missing or erroneous data are two of the most important issues when modelling using neural network techniques, as discussed in chapter 4.
<table>
<thead>
<tr>
<th>Element</th>
<th>Total Data</th>
<th>Training Data</th>
<th>Test Data</th>
<th>Validation Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>316</td>
<td>125</td>
<td>125</td>
<td>66</td>
</tr>
<tr>
<td>B</td>
<td>299</td>
<td>125</td>
<td>125</td>
<td>49</td>
</tr>
<tr>
<td>C</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>Ca</td>
<td>206</td>
<td>75</td>
<td>75</td>
<td>56</td>
</tr>
<tr>
<td>Cr</td>
<td>317</td>
<td>125</td>
<td>125</td>
<td>67</td>
</tr>
<tr>
<td>Cu</td>
<td>317</td>
<td>125</td>
<td>125</td>
<td>67</td>
</tr>
<tr>
<td>Mn</td>
<td>326</td>
<td>125</td>
<td>125</td>
<td>76</td>
</tr>
<tr>
<td>Mo</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>N</td>
<td>317</td>
<td>125</td>
<td>125</td>
<td>67</td>
</tr>
<tr>
<td>Nb</td>
<td>317</td>
<td>125</td>
<td>125</td>
<td>67</td>
</tr>
<tr>
<td>Ni</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>O</td>
<td>230</td>
<td>85</td>
<td>85</td>
<td>60</td>
</tr>
<tr>
<td>P</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>S</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>Si</td>
<td>325</td>
<td>125</td>
<td>125</td>
<td>75</td>
</tr>
<tr>
<td>Ti</td>
<td>315</td>
<td>125</td>
<td>125</td>
<td>65</td>
</tr>
<tr>
<td>V</td>
<td>317</td>
<td>125</td>
<td>125</td>
<td>67</td>
</tr>
</tbody>
</table>

**Table 5.1** – Data quantities for the weld chemistry parameters considered for neural network modelling
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Max</th>
<th>Min</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wire Ni wt.%</td>
<td>2.410</td>
<td>0.017</td>
<td>0.272</td>
</tr>
<tr>
<td>Weld Ni wt.%</td>
<td>1.220</td>
<td>0.020</td>
<td>0.243</td>
</tr>
<tr>
<td>Plate Al wt.%</td>
<td>0.099</td>
<td>0.007</td>
<td>0.036</td>
</tr>
<tr>
<td>Wire Al wt.%</td>
<td>0.039</td>
<td>0.005</td>
<td>0.018</td>
</tr>
<tr>
<td>Weld Al wt.%</td>
<td>0.040</td>
<td>0.007</td>
<td>0.022</td>
</tr>
<tr>
<td>Plate Ti wt.%</td>
<td>0.020</td>
<td>0.001</td>
<td>0.006</td>
</tr>
<tr>
<td>Wire Ti wt.%</td>
<td>0.150</td>
<td>0.001</td>
<td>0.064</td>
</tr>
<tr>
<td>Weld Ti wt.%</td>
<td>0.040</td>
<td>0.000</td>
<td>0.014</td>
</tr>
<tr>
<td>Plate P wt.%</td>
<td>0.018</td>
<td>0.005</td>
<td>0.011</td>
</tr>
<tr>
<td>Wire P wt.%</td>
<td>0.023</td>
<td>0.006</td>
<td>0.012</td>
</tr>
<tr>
<td>Weld P wt.%</td>
<td>0.024</td>
<td>0.009</td>
<td>0.015</td>
</tr>
<tr>
<td>Plate S wt.%</td>
<td>0.010</td>
<td>0.001</td>
<td>0.004</td>
</tr>
<tr>
<td>Wire S wt.%</td>
<td>0.011</td>
<td>0.002</td>
<td>0.008</td>
</tr>
<tr>
<td>Weld S wt.%</td>
<td>0.014</td>
<td>0.002</td>
<td>0.006</td>
</tr>
<tr>
<td>Plate N wt.%</td>
<td>0.016</td>
<td>0.002</td>
<td>0.005</td>
</tr>
<tr>
<td>Wire N wt.%</td>
<td>0.010</td>
<td>0.003</td>
<td>0.007</td>
</tr>
<tr>
<td>Weld N wt.%</td>
<td>0.014</td>
<td>0.004</td>
<td>0.007</td>
</tr>
<tr>
<td>Plate O wt.%</td>
<td>0.012</td>
<td>0.001</td>
<td>0.003</td>
</tr>
<tr>
<td>Wire O wt.%</td>
<td>0.022</td>
<td>0.000</td>
<td>0.001</td>
</tr>
<tr>
<td>Weld O wt.%</td>
<td>0.048</td>
<td>0.021</td>
<td>0.030</td>
</tr>
<tr>
<td>Acicular Ferrite (AP%)</td>
<td>99.300</td>
<td>60.500</td>
<td>86.474</td>
</tr>
<tr>
<td>Primary Ferrite (PF%)</td>
<td>32.000</td>
<td>0.600</td>
<td>12.536</td>
</tr>
<tr>
<td>Ferrite Side-plate (FS%)</td>
<td>36.300</td>
<td>0.000</td>
<td>0.991</td>
</tr>
<tr>
<td>Average Impact Energy 60°C</td>
<td>186.000</td>
<td>121.000</td>
<td>148.875</td>
</tr>
<tr>
<td>Average Impact Energy 40°C</td>
<td>190.000</td>
<td>115.000</td>
<td>150.156</td>
</tr>
<tr>
<td>Average Impact Energy 20°C</td>
<td>211.000</td>
<td>16.000</td>
<td>145.024</td>
</tr>
<tr>
<td>Average Impact Energy -10°C</td>
<td>211.000</td>
<td>40.000</td>
<td>136.176</td>
</tr>
<tr>
<td>Average Impact Energy -20°C</td>
<td>170.000</td>
<td>25.000</td>
<td>97.346</td>
</tr>
<tr>
<td>Average Impact Energy -30°C</td>
<td>202.000</td>
<td>27.000</td>
<td>112.691</td>
</tr>
<tr>
<td>Average Impact Energy -50°C</td>
<td>196.000</td>
<td>10.000</td>
<td>79.726</td>
</tr>
<tr>
<td>Average Impact Energy -70°C</td>
<td>195.000</td>
<td>13.000</td>
<td>57.423</td>
</tr>
<tr>
<td>Average Impact Energy -90°C</td>
<td>156.000</td>
<td>10.000</td>
<td>41.920</td>
</tr>
<tr>
<td>Average Impact Energy -110°C</td>
<td>99.000</td>
<td>7.000</td>
<td>30.244</td>
</tr>
<tr>
<td>Average Impact Energy -130°C</td>
<td>154.000</td>
<td>8.000</td>
<td>34.000</td>
</tr>
</tbody>
</table>

Table 5.2 - Data distribution for information used in modelling weld metal chemistry, microstructure, mechanical properties and weld bead geometry
5.2.2 Statistics on data

The range of information covered by the data used in training a neural network has a strong influence on the ability of the model to generalise well. Information as to the range of data used for modelling chemistry, mechanical properties and weld bead geometry in this thesis is summarised in Table 5.2. The quantity of data depends on the different properties being modelled, and decreases with increasing number of inputs and outputs due to the need for complete, clean and robust data.

From previous work carried out at Loughborough University\textsuperscript{90}, it was found that for a single output model more complex neural networks, considering a larger number of weld process parameters had no benefit over simpler lower input models when considering the weld metal chemistry of each element in turn. Later studies described further on in this chapter, show that using a larger number of inputs and outputs, a multiple output model, enables the complex reactions between alloying elements to be mapped far more accurately, enabling predictions of the eventual overall weld metal chemistry to a higher standard.

Early work utilising the data in Table 5.1 to model weld metal chemistry considered a simple 5-input model, varying the number of hidden units as an evaluating factor. The 5 inputs considered were plate thickness, heat input, wire stickout and plate and consumable concentration of the element X. All neural network modelling of weld metal chemistry described in this section uses just 100 Markov chain Monte Carlo steps, which was thought to be the most computationally efficient number for the data being mapped.

5.3 Discussion and results from early neural network modelling of weld metal chemistry

Predictions of certain elements were found to be better than others using the data described above. Analysis of the results will therefore consider a good predictive model in comparison with a model, which predicted data relatively poorly, representing the results achievable with neural network modelling. Results from modelling of other elements in weld metal chemistry can be found in appendix II section 1.
5.3.1 Titanium

A five input architecture was used in the modelling of titanium, varying the number of nodes in the hidden layer from 1 hidden unit (considered a linear model) through to 9, using 100 chains for each model. The average mean squared error plotted against the number of hidden units is used as an evaluation of the accuracy of the neural network models. A plot of this can be seen in Figure 5.1 and the data are summarised in Table 5.3. Evaluation of the training and test errors show that testing has a greater error than training. This is to be expected because the test data show the model handling previously unseen data after training has taken place. The training error can generally be expected to be lowered in most cases when more Markov chain Monte Carlo steps are used, although the compromise between computing time and gain in model accuracy must be weighed up.

![Graph showing the average mean squared error against the number of hidden units used for a neural network model of weld metal titanium content](image)

Figure 5.1 – Graph showing the average mean squared error against the number of hidden units used for a neural network model of weld metal titanium content

From the graph in Figure 5.1 of average squared error against the number of hidden units, it would be expected that the accuracy of predictions of models using higher numbers of hidden units is the greatest. Figures 5.2 and 5.3 showing predictions for network architectures with 1 and 9 hidden units respectively confirm this hypothesis. Ideally all points on a graph of predicted data against actual data should sit on a line ‘y = x’, and by considering this line on the two graphs Figure 5.2 and 5.3, we see that the 9 hidden unit neural network model of titanium weld chemistry is the most accurate.
Neural Network Modelling of Weld Metal Chemistry and Microstructure

<table>
<thead>
<tr>
<th>Number of Hidden Units</th>
<th>Average Sum Squared Error in Training</th>
<th>Average Sum Squared Error in Testing</th>
<th>Average Sum Squared Error for all Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.123</td>
<td>0.136</td>
<td>0.130</td>
</tr>
<tr>
<td>3</td>
<td>0.063</td>
<td>0.107</td>
<td>0.085</td>
</tr>
<tr>
<td>5</td>
<td>0.052</td>
<td>0.081</td>
<td>0.067</td>
</tr>
<tr>
<td>7</td>
<td>0.050</td>
<td>0.081</td>
<td>0.066</td>
</tr>
<tr>
<td>9</td>
<td>0.048</td>
<td>0.079</td>
<td>0.064</td>
</tr>
</tbody>
</table>

Table 5.3 – Table summarising the average sum squared error for training, test and total data sets for the titanium neural network models.

Figure 5.2 – Plot of predicted points, made using validation data, against actual data for titanium weld chemistry prediction using a 5 input model with 1 hidden unit
Neural Network Modelling of Weld Metal Chemistry and Microstructure

Figure 5.3 – Plot of predicted points, made using validation data, against actual data for titanium weld chemistry prediction using a 5 input model with 9 hidden units

5.3.2 Sulphur

Figure 5.4 – Graph showing the average mean squared error against the number of hidden units used for a neural network model of weld metal sulphur content

A different behaviour is presented in the sulphur case using a 5 input neural network model. In Figure 5.4 the average sum squared error as a function of the number of hidden units is shown graphically. In this case the trend is quite different from that of the titanium model; there is less of a downward trend in the average sum squared error as more hidden units are added, especially where the overall and test errors are considered. Additionally the magnitude of error is far higher
Neural Network Modelling of Weld Metal Chemistry and Microstructure

for the modelling of weld metal sulphur content, compared with titanium. This is reflected in the prediction of the sulphur weld chemistry. Unlike the titanium model, there is no significant difference between the 1 hidden unit model and the 9 hidden unit model, shown in Figures 5.5 and 5.6 respectively. When comparing with the ‘$y = x$’ line there is no distinct difference in the predictive capability of either model. There are several reasons for this; firstly there is a low variation in the data used for training the network, in respect of plate and wire sulphur content, therefore the model is poor at generalising when presented with previously unseen data. Secondly, more chains may be needed in the modelling of sulphur chemistry compared with titanium chemistry to achieve sufficient equilibrium in the model, thus with more calculations being used per step a more accurate learning process is evolved and eventually will be reflected in an improved prediction of results.

![Figure 5.5](image_url)

**Figure 5.5** - Plot of predicted data against actual data for sulphur weld chemistry prediction using a 5 input model with 1 hidden unit - made using validation data
Neural Network Modelling of Weld Metal Chemistry and Microstructure

Figure 5.6 - Plot of predicted data against actual data for sulphur weld chemistry prediction using a 5 input model with 9 hidden units - made using validation data

The plots for both titanium prediction and sulphur prediction are shown with error bars calculated by the network. The error is representative of one standard deviation and can be derived using equation 4.9.

\[ sd = \sqrt{\frac{\sum (t-o)^2}{N-1}} \]  \hspace{1cm} 4.9

where ‘\( o \)’ is the mean value predicted, ‘\( x \)’ is the real value input and \( N \) is the number of predictions made. From both graphs of titanium and sulphur, it is observed that errors are greater in the sulphur model, due to the error in both training and testing leading to a badly trained network in comparison to the titanium model.

5.3.3 Comparison with linear regression techniques

Linear regression models have been developed by Thewlis et al of Corus\(^89\) using the same data considered in the neural network modelling of weld metal chemistry described in this chapter.
For comparative purposes with the neural network model for weld metal Ti content shown in Figure 5.3, Figure 5.7 presents an example of the linear regression analysis taken from work carried out by Thewlis et al.\(^\text{89}\). It is clearly visible by considering the \( y = x \) ideal line, that the linear regression analysis is poorer at predicting accurate results when compared with neural network models. The assumptions required for linear regression modelling simplify the relationship between input chemical elements and eventual chemistry of the weld, missing essential complex chemical reaction phenomena. Without information as to the content of other input elements modelling of these complex phenomena is impossible, even with the ‘black-box’ capabilities of a neural network model. The neural network techniques are better utilised with more complex relationships such as weld metal properties, and modelling where multiple outputs are required; thus requiring far more inputs to model accurately.

5.4 Development of modelling techniques for the prediction of weld metal chemistry

The modelling of weld metal chemistry described in the previous section considered only a single element at a time. Vital relative information with regards to other influential alloying elements is therefore not considered. The possibility of combining the information from several models, and creating an output for all elements in the weld metal is therefore attractive as more
complex rules and interactions can be considered. To enable such a complex mapping of the data normalisation between \(-0.5\) and \(0.5\) is utilised which was found to improve relative neural network performance. Normalisation to zero mean and standard deviation equal to 1 as used in the early chemistry work was found to yield poor results. The reasoning behind why different scaling techniques yield better results has been discussed in chapter 4, section 4.4.1.

The underlying intention in this work is to incorporate various models together, for example to link chemistry and toughness, and therefore weld metal chemistry outputs were selected carefully to cut down the number of outputs required and to set a limit to the amount of repeat modelling being considered. The chemistry of only the outer diameter welds was considered. The chemical elements considered are; carbon (C), manganese (Mn), silicon (Si), aluminium (Al), phosphorus (P), sulphur (S), nitrogen (N), oxygen (O). Additionally separate models for each chemical element were also developed as a comparison with both multiple and single output architectures because of the different scaling range used in this work.

Once information for outer diameter welds was filtered from the complete database, thorough examination and cleaning was undertaken. This pre-processing yielded 135 data rows, once the multiple output modelling structure was taken into consideration. It was decided to use these same data for both multiple and single output modelling to give a clear comparison between each type of modelling architecture. Once normalised the data was randomised and split into two forming 70 data pairs for training and 65 data pairs for testing. The modelling process undertaken used 1000 Markov chain Monte Carlo steps to give the neural network sufficient computing time to converge.

5.4.1 Single output weld metal chemistry modelling – Normalisation scaled from \(-0.5\) to \(+0.5\)

Consistent with earlier work neural network models were developed keeping inputs and outputs constant using the number of hidden units as the evaluative modelling parameter. All inputs except one were kept the same as the early modelling described in section 5.2, however wire stickout was replaced by the welder speed as this was considered more relevant through the modelling activities undertaken in this work. Therefore, model architectures took the following form:
Neural Network Modelling of Weld Metal Chemistry and Microstructure

Inputs

- Plate thickness (mm)
- Weld travel speed (mm/min)
- Measured heat input (kJ/mm)
- Plate wt.% of element X prior to welding
- Wire wt.% of element X

Output

- Weld wt.% of element X

Results from modelling showed an improvement on the work done previously normalising data to zero mean and standard deviation equal to 1, which was noticeable across the whole range of elements but particularly for elements O and P. The training and test errors are presented in appendix II section 2, however, the results showed a very flat response for a varying number of hidden units across the range of elements. This much smaller variation in error between models of different architectural complexity is explained by the use of the narrower scale of normalisation; the data having scaling limits well inside the finite limits of the activation function. Figure 5.8 (a-h) are the predictions for each element across the training data domain, and Figure 5.9 (a-h) the predictions for each element across the test data domain for the optimum neural network architecture for each weld metal chemistry model. Comparing results obtained in section 5.3 with the work in this section showed that normalisation between -0.5 and 0.5 is far better when modelling weld metal chemistry in contrast to normalising to a zero mean and standard deviation equal to one, with training and test errors being far less and thus reflecting in the predictions being made.

5.4.2 Input relevance – Comparison between both methods of normalisation for weld metal chemistry

From the results already considered for modelling weld metal chemistries in section 5.2 and 5.4.1, normalisation of the data between the limits -0.5 to 0.5 yields far better results, noticeable both with errors in training and testing and also when making predictions. In order to support the findings of the work in section 5.4.1, an investigation of the weights placed on the connections from each input was undertaken to determine how the neural network models are forming the rules around the data compared to expectations from prior metallurgical knowledge. Data for all neural network models for each individual chemical element has been examined, although for
the purpose of this chapter the element aluminium (Al) is considered specifically, and all other results can be found in appendix II, section 3.

As a comparison of the predictions made using different data scaling techniques, the graph in figure 5.10 shows the predictions made using validation data for weld metal aluminium content normalised to zero mean and standard deviation equal to 1. The neural network architecture used in this case contained 9 hidden units, whereas in figure 5.8 and 5.9 (d) a 7 hidden unit architecture was used with data being normalised between -0.5 and 0.5. A comparison of the predictions made shows that the -0.5 and 0.5 scaling technique yields results fitting the 'y=x' situation much closer, and furthermore the size of the error bars being far smaller.
Fig. 5.8 – Predictions made using optimum neural network architectures for weld metal chemistry prediction of element X, across the training data domain. (a) Weld wt.% C – 7 Hidden units, (b) Weld wt.% Mn – 5 Hidden units (c) Weld wt.% Si – 9 Hidden units, (d) Weld wt.% Al – 7 Hidden units, (e) Weld wt.% P – 7 Hidden units, (f) Weld wt.% S – 9 Hidden units, (g) Weld wt.% N – 7 Hidden units, (h) Weld wt.% O – 9 Hidden units.
Fig. 5.9 - Predictions made using optimum neural network architectures for weld metal chemistry prediction of element X, across the test data domain. (a) Weld wt.% C - 7 Hidden units, (b) Weld wt.% Mn - 5 Hidden units (c) Weld wt.% Si - 9 Hidden units, (d) Weld wt.% Al - 7 Hidden units, (e) Weld wt.% P - 7 Hidden units, (f) Weld wt.% S - 9 Hidden units, (g) Weld wt.% N - 7 Hidden units, (h) Weld wt.% O - 9 Hidden units
Figure 5.10 – Predictions made using validation data for a neural network modelling weld metal Al content containing 9 hidden units, using data normalised with mean and standard deviation

Information retrieved from respective neural network models as to the weighting placed on each individual input was evaluated as to which model is fitting the data as would be expected from prior metallurgical knowledge. Figures 5.11 (a) and (b) show the perceived significance, $\sigma_w$, placed on the connections between inputs and output, for scaling between the limits $-0.5$ to $0.5$ and normalising to zero mean and standard deviation equal to $1$ respectively, with $\sigma_w$ for input connections to hidden layer for each individual parameter being displayed in Figure 5.12 (a) and (b) respectively. It can be seen from these figures that the model has mapped the data as would be expected from prior metallurgical knowledge. The largest influence is seen to be placed on plate and wire content of Al, with plate thickness also shown to carry some influence, which is expected as it is related to dilution factors. The model using data normalised to zero mean and standard deviation equal to one, shows larger weightings across the input to hidden connections on weld input parameters rather than chemistry, placing most influence upon the plate thickness and the wire stickout. This evidence confirms that the modelling of weld metal chemistries using data normalised between the limits $-0.5$ and $0.5$ is most accurate; following the rules that would be expected from knowledge of the welding process.
Figure 5.11 (a) – Perceived significance, $\sigma_w$, between input and output layer for each individual input parameter, for a neural network containing 7 hidden units modelling data for weld metal Al chemistry normalised between -0.5 and 0.5

Figure 5.11 (b) – Perceived significance, $\sigma_w$, between input and output layer for each individual input parameter, for a neural network containing 9 hidden units modelling data for weld metal Al chemistry normalised to have zero mean and standard deviation equal to 1
Figure 5.12 (a) – Perceived significance, $\sigma_w$, between input and hidden layer for each individual input parameter, for a neural network containing 7 hidden units modelling data for weld metal Al chemistry normalised between −0.5 and 0.5

Figure 5.12 (b) – Perceived significance, $\sigma_w$, between input and hidden layer for each individual input parameter, for a neural network containing 9 hidden units modelling data for weld metal Al chemistry normalised to have zero mean and standard deviation equal to 1
5.4.3 Multiple output neural network model for weld metal chemistry

When considering the contribution of each chemical element input into the weld pool, be it from welding wire or the parent plate, to the final weld metal chemistry, it is important to consider their interaction during the complex high speed reactions taking place during a high temperature thermal cycle. Therefore a multiple output neural network model taking into account the eventual weld metal chemistry of several chemical elements was developed considering the full range of plate and wire chemistries for the modelled weld metal outputs. With future work also in mind, specifically the forward feeding of outputs to the input layer of a neural network model for weld metal toughness, the elements chosen were as represented in section 5.3.1. The neural network architectures are described below, with varied numbers of nodes within the hidden layer again being used as the evaluative modelling parameter:

**Inputs**
- Plate Thickness (mm)
- Welder Travel Speed (mm/min)
- Measured Heat Input (kJ/mm)
- Plate wt.% C
- Wire wt.% C
- Plate wt.% Mn
- Wire wt.% Mn
- Plate wt.% Si
- Wire wt.% Si
- Plate wt.% Al
- Wire wt.% Al
- Plate wt.% P
- Wire wt.% P
- Plate wt.% S
- Wire wt.% S
- Plate wt.% N
- Wire wt.% N
- Plate wt.% O
- Wire wt.% O

**Outputs**
- Weld wt.% C
- Weld wt.% Mn
- Weld wt.% Si
- Weld wt.% Al
- Weld wt.% P
- Weld wt.% S
- Weld wt.% N
- Weld wt.% O
As previously described in section 5.4.1, 135 data were made available for the training and test processes and due to the small quantity of data available a validation set was not made available. Data were normalised between the limits \(-0.5\) and \(0.5\), as this proved to be most successful from the previous work in this chapter and once normalised the data was randomised and split, forming 70 data rows for training and 65 data rows for testing. The training and test processes were undertaken using 1000 Markov Chain Monte Carlo steps so as to provide sufficient converging of results for the more complex architectures containing high numbers of nodes within the input, hidden and output layers.

![Figure 5.13](image_url)

**Figure 5.13** – Error on training and testing process for a multiple output neural network model for weld metal chemistry

Little variation was seen in the training and testing process, though once again this is explained by the scaling of the data between \(-0.5\) and \(+0.5\) compared with the activation function employed having finite limits between \(-1\) and \(+1\). The training and test error shown in Figure 5.13, evaluated the varied number of hidden units up to a total of 13 because beyond this number the models would require far more Markov chain Monte Carlo steps. The use of an increased number of Markov chain Monte Carlo steps alongside a greater number of hidden units above 13 was felt to be unnecessary and inefficient as far as computing time is concerned and therefore results are omitted. The optimum number of hidden units was found to be 8, and the results of the application of this optimum model for predictions made across the training and test data domain are shown in Figure 5.14 (a-h) and Figure 5.15 (a-h) respectively.
Fig. 5.14 – Predictions made using optimum neural network architectures for weld metal chemistry prediction of element X, across the training data domain using a multiple output neural network model for weld metal chemistry, with architecture containing 8 hidden units. (a) Weld wt.% C, (b) Weld wt.% Mn, (c) Weld wt.% Si, (d) Weld wt.% Al, (e) Weld wt.% P, (f) Weld wt.% S, (g) Weld wt.% N, (h) Weld wt.% O.
Fig. 5.15 - Predictions made using optimum neural network architectures for weld metal chemistry prediction of element X, across the test data domain using a multiple output neural network model for weld metal chemistry, with architecture containing 8 hidden units. (a) Weld wt.% C, (b) Weld wt.% Mn, (c) Weld wt.% Si, (d) Weld wt.% Al, (e) Weld wt.% P, (f) Weld wt.% S, (g) Weld wt.% N, (h) Weld wt.% O.
Fig. 5.16 - Weights on connections from inputs for each individual output parameter, for a multiple output neural network modelling data for weld metal chemistry normalised between the limits -0.5 and 0.5 containing 8 hidden units. (a) wt.% C (b) wt.% Mn (c) wt.% Si (d) wt.% Al (e) wt.% P (f) wt.% S (g) wt.% N (h) wt.% O
The results of predictions made across the training and test data domains show a significant improvement on those in both previous attempts using separate neural network models for each chemical element. The most visible improvement is seen on the training data for wt.% O, in which the predictions are seen to fit the $y = x$ relationship between actual and predicted points far better. The improvement in predictions is attributed to the complex alloying phenomena that take place giving the neural network a wider spread of information to consider across the range of chemical elements being input to the weld metal. A larger number of modelling inputs enables more complex rules governing the relationship between welding parameters, plate chemistries and wire chemistries with the eventual weld metal chemistry to be formed.

5.4.4 **Input relevance – multiple output model**

An investigation into weightings placed on the connections from each individual input between the layers qualifies the ability of the model to create rules governing the mapping between inputs and outputs across the data space. Information gathered about these weightings allows a comparison for each chemical element individually in modelling the overall weld metal chemistry. In these modelling trials multiple output architectures are being examined and therefore in an attempt to validate the results the weights on the connections from each individual input to each output were examined. Results shown in Figure 5.16 (a-h) are the weightings across the range of outputs for each individual input parameter; average values across the neural network models can be found in appendix II, section 4. The average for the weights across the connections between input and hidden layer are shown in Figure 5.17, in which these weightings describe the influence of the input parameters for the more complex relationships found within the data domain.

From the results seen in Figure 5.16, considering each output parameter individually, it is observed that the neural network model has formed the rules well with regards each individual output parameter. The wt.% of each individual element X in the plate and/or wire has the highest influence when considering the amount of that particular element X in the weld metal, as would be expected. The weld metal phosphorus and weld metal oxygen do not show the expected behaviour due to the more complex reactions involved with these two elements. By considering an average across the whole domain of outputs, represented graphically in appendix II section 4, there is no clear indication as to the biggest influencing parameter, however, due to the many complex reactions taking place it is not expected that a singular influential factor would exist. Welder speed
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is seen to carry a relatively high weighting, compared to other welding process parameters across the input to output weight space. The welder speed is directly related to the deposition rate of weld metal from welding wires, to a given point in the welding run, and therefore would be directly related to the deposition of the individual alloying elements being modelled here. More complex relationships are identifiable through an investigation of weightings placed on the connections between input and hidden layer, as shown in Figure 5.17. Manganese (Mn), silicon (Si), phosphorus (P), sulphur (S) and nitrogen (N) are featured highly in the weighting, with very little influence being placed on welding control parameters.

Figure 5.17 - Average weights between input and hidden layer for each individual input parameter, for a multiple output neural network modelling data for weld metal chemistry normalised between the limits -0.5 and 0.5

5.5 – Discussion of the results of neural network modelling of weld metal chemistry

Phosphorus, sulphur and nitrogen are considered as impurities that are not only responsible for the decrease in fracture toughness of the weld metal but are known to form as inclusions once alloyed with other input chemical additions. The high influence of such impurities is expected to have an effect on all other alloying reactions taking place, as other modelled elements are put into the chemical mix to remove these so called impurities. For example titanium is added as a micro-alloying element, mainly as a means of tying up any free nitrogen, while calcium is used in a
similar way in the reduction of sulphur content in the final weld metal chemistry. Therefore the high weighting on these so-called impurities would be expected, as there is a strong relationship between their presence in plate and wire content, and the eventual content of these impurities and other alloying elements in the final weld metal chemistry.

Manganese is the most common weld alloying element after carbon and is generally found in all steels, being a strong alloying element it has a large influence on the form that other chemical elements that will be found in the weld metal. For example galaxite, MnOAl₂O₃, is found in abundance in the form of inclusions throughout the weld metal microstructure of steel line-pipe. Manganese along with silicon are both known to be used as part of the de-oxidation process, this usage stemming from theory developed for steel making. The ratio of manganese to silicon is balanced so as to obtain non-saturated manganese silicates, giving the best possible de-oxidation. Therefore the presence of these two alloying elements is fundamental to the welding of a sound join, and is of no surprise that a substantial influence is placed upon these alloying chemistries by the neural network.
5.6 A neural network model to predict the weld metal microstructure

When considering the mechanical properties of the weld metal, it is useful to know the type of metallurgical structure that has been formed during the welding process. This metallurgical structure is directly related to the mechanical properties and hence the quality of the weld. A possible method of attack to the problem of modelling weld metal toughness from weld process parameters and consumable inputs, is to consider the constituents found within the weld metal microstructure, specifically considering the percentage of acicular ferrite within the weld metal. The acicular ferrite content of a weld is directly linked to its toughness. The eventual microstructure of the weld metal is related to the chemical input and the thermal cycle created during the welding and cooling processes. From the data used in modelling, the cooling rate was not described in a sufficient manner and therefore an alternative method was required.

The acicular ferrite phase is most commonly observed during the cooling of low alloy steel weld deposits as part of the austenite transformation. Formation of acicular ferrite usually occurs in the temperature range where re-constructive transformations become relatively slow, giving way to displacive reactions such as formation of Widmanstätten ferrite, bainite and martensite. In an effort to evaluate the best method, a single output model for acicular ferrite (AF%) and a multiple output model considering percentage acicular ferrite (AF%), primary ferrite (PF%) and ferrite side-plate (FS%) were developed.

5.6.1 Single output model for acicular ferrite content

In the initial modelling architecture for weld metal toughness as described in chapter 7.1, the use of acicular ferrite as a modelling parameter was key to successfully making accurate predictions. In a manufacturing environment information as to the levels of microstructural constituents are not readily available, especially before the weld has been made, and therefore prediction of the weld metal content from welding parameters is an important step towards accurate prediction of weld metal toughness from welding process parameters. As a starting point for the modelling of the weld metal microstructure a single output model for weld metal acicular ferrite was initially developed considering chemical composition and weld process parameters related to the thermal cycle. The input architecture contained 18 inputs for the single output AF% model; the number of
hidden units was varied so as to evaluate the best neural network model. The inputs were as follows:

- Plate thickness
- Welder travel speed
- Combined heat input
- Wire vertical stickout
- Spacing wire 1 to wire 2
- Spacing wire 2 to wire 3
- Weld wt.% C
- Weld wt.% Mn
- Weld wt.% Cr
- Weld wt.% Mo
- Weld wt.% Si
- Weld wt.% Ni
- Weld wt.% Al
- Weld wt.% Ti
- Weld wt.% P
- Weld wt.% S
- Weld wt.% N
- Weld wt.% O

Following pre-processing of the data a total of 173 data sets were available for the modelling process. Normalisation between the limits -0.5 and 0.5 was undertaken before the data were randomised and split into a training set, 82 data, test set, 82 data, and validation set, 9 data. An evaluation of the average sum square error compared with the increased complexity of the neural network architecture is shown in Figure 5.18, revealing the best neural network architecture to contain 10 hidden units. It was also observed that the models containing 14-16 hidden units had not reached equilibrium, though increases in the number of Markov chain Monte Carlo carries the large negative of increasing computing time considerably.

Predictions made on training, test and validation data are compared in Figure 5.19 plotting all points of actual AF% against predicted AF% and comparing with the ‘y=x’ ideal line. It is seen from the plot of predictions made across the training data domain that the neural network has formed the rules around the data well, and although the predictions made across the test data, and validation data show an increase in the amount of error, though there is good correlation with the expected y = x relationship. Some outliers are seen in the predictions made across the test data domain which is a result of the fact that the data present in the training and test data domains does not quite overlap and thus is not predicted quite so accurately. This problem would be overcome if more data were available enabling a larger number of modelling scenarios to form the rules around the data.
Figure 5.18 – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of weld metal acicular ferrite content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs.

Figure 5.19 – Comparison of predictions made using training, test and validation data for a neural network model for weld metal acicular ferrite content, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs.

Perceived significance, \( \sigma_{w} \), results for both input to output and input to hidden layer are seen in Figure 5.20, and show a strong weighting is placed on the input parameters wt.% Al and wt.%
Ti, these two elements are found to be present in high quantity in the form of inclusions within the line-pipe weld metal being modelled. An experimental investigation of line-pipe weld metallurgy has been presented in chapter 3, in which it was concluded that these inclusions were found to perform as nucleation sites for acicular ferrite and long ferrite laths. Other inputs showing a relatively large level of influence are heat input, plate thickness and various alloying elements including Cr, Mn and C. These would all be expected as the heat input and plate thickness are indicators as to the thermal cycle applied to the weld metal, while chemical elements play a major role in the alloying and therefore transformation kinetics within the steel. A good correlation between the rules being formed by the neural network around the data, and what would be expected from prior metallurgical knowledge is therefore seen through the examination of the $\sigma_w$ values.

Figure 5.20 (a) - Perceived significance, $\sigma_w$, for connections between input and output layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs
5.6.2 Multiple output model for weld metal microstructure – with the aim of predicting acicular ferrite content

With the aim of improving the previously developed modelling architecture, the use of a three-output model was considered using the same input architecture as that of the AF% model while mapping to the following three outputs:

- Weld metal % acicular ferrite (AF%)
- Weld metal % primary ferrite (PF%)
- Weld metal % ferrite side plate (FS%)

It was hoped that the relationship between outputs would enhance the predictive capabilities of the neural network model while maintaining the same input parameters following a similar procedure to that seen in the modelling of weld metal chemistry earlier in this chapter. As with the previous modelling, data were normalised between the limits -0.5 and 0.5 and randomised.
before splitting into training, test and validation sets, in the same proportions as designated in the previous section. Errors across the training and testing phase, for increased model complexity are shown in Figure 5.21, which highlights the rapid decrease of the training error to near zero. This rapid fall in training error to these extremely low levels is an indicative sign of the model overfitting the data presented to it.

\[
\begin{align*}
W & \sim 0.10 \\
\sigma & \sim 0.08 \\
\end{align*}
\]

\[
\begin{align*}
\text{Figure 5.21} & \quad \text{Average sum squared error shown with increasing complexity of the neural network architecture for a multiple output neural network modelling weld metal microstructure content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs.}
\end{align*}
\]

An investigation into the errors across training and testing phases showed the best neural network architecture to contain 10 hidden units. For a 10 hidden unit neural network training error is not seen to significantly change when compared to simpler or more complex architectures, although the test error was found to carry an optimum error level without any linked rise in the training error. Predictions made across the training, test and validation data domains are compared in Figures 5.22 (a-c). It is clear that from the near zero training error that as expected predictions on the training data domain fit the \( y = x \) relationship between actual and predicted points almost exactly for all three separate microstructure constituents.
Figure 5.22 – Comparison of predictions made using training, test and validation data for a multiple output neural network model predicting (a) weld metal % AF content, (b) weld metal % PF content and (c) weld metal % FS content, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs.

Observing the predictions made across the testing and validation domains, Figure 5.22 (b) and (c), it can be seen that the error bars are relatively large on some cases and small on others, due to the overfitting that has taken place during the training phase. Variation in data for weld metal ferrite side-plate content, FS%, is small, therefore the level of confidence in the modelling generalisation for FS% is low. The rules governing the neural network output are poor and do not generalise well, therefore only a fraction of data being considered are predicted well.
Comparing predictions of weld metal acicular ferrite content, the most desirable output parameter, a fall in performance is noticed in contrast to that of the model described in the previous section. This fall in performance is attributed to the added complexity of the new modelling architecture, the results not following the trend seen in modelling of weld metal chemistry.

In order to evaluate the model further, investigation into the weightings being placed on connections between inputs and hidden layer, and inputs and each individual output were considered. The input to output layer weightings are displayed in Figure 5.23(a) to (c) for AF%, PF% and FS% respectively, whilst the average weightings across the net from input to hidden layer are shown in Figure 5.24.

Weights on input to output layer connections in Figure 5.23 show the highest weighting to be placed upon the welder travel speed. Welder travel speed is directly related to the heat input to the weld pool; a faster travel speed reduces the energy applied at a given point in the welding run. Comparing the relative weighting placed on the welder travel speed input parameter for each output parameter it is seen to play a considerable role in the formation of the rules around the modelling data, with all other inputs showing little weighting in comparison.

Examination of the input to hidden layer connections, shown in Figure 5.24, reveals a wider distribution of the weightings placed on the input parameters with no clear determining variable. The influence is seen to shift from welder travel speed to the more complex weld metal chemistries key to the formation of the weld metal microstructure. Relatively high weightings are placed on the elements Mo, Ti, Al, Ni, Si and Mn whereas the welding process parameters show very little relative weighting. Molybdenum and Manganese can be considered as being influential on the austenite to ferrite transformation, and for the formation of a fine grain structure; important to the manufacture of welds with good toughness properties. Titanium and aluminium have been shown to be present in inclusions paramount to the nucleation of acicular ferrite microstructure.
Typically an arc-weld contains a quantity of inclusions of the order of $10^{18}$ m$^{-3}$, and of a size greater than 0.05 μm distributed throughout the microstructure. The entrapment of complex multi-phase non-metallic inclusions in the solid weld metal is caused through the interaction of the liquid weld metal with surrounding gases, together with the use of strong de-oxidising elements such as silicon, aluminium and titanium. The inclusions have two major effects on the steel; they serve as nucleation sites promoting growth of intragranular acicular ferrite leading to increased toughness without loss in strength. Nucleation voids during ductile fracture and nucleation of cleavage cracks during brittle fracture are also caused by the presence of these...
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It is important to achieve a good balance between these conflicting factors; a difficult task without a basic understanding of the mechanisms driving these interactions.

Figure 5.24 – Average weights on connections across the net from each input parameter to hidden layer, for each output parameter for a neural network model with 10 hidden units modelling weld metal microstructure

Results throughout the literature prove that for heterogeneous nucleation of acicular ferrite the inclusions responsible must be inhomogeneous. Bhadeshia\textsuperscript{88} makes reference to the various phases found within such inclusions, detailing the complex layers of nitrides, sulphides and oxides seen to make-up these nucleation sites. Thermodynamic arguments are also put forward that seem to contradict the complex inclusion structures. Taking assumptions found in classical nucleation theory it has been demonstrated that inclusions are less effective in nucleating ferrite when compared with austenite grain surfaces\textsuperscript{117}. Bhadeshia's\textsuperscript{88} work on the modelling of microstructure evolution in steel welds details the energy theory behind the nucleation of ferrite favouring austenite grain surfaces.

The highly complex nature of inclusions and the difficulty encountered in conducting controlled welding experiments means that the nucleation potency of the various inclusions types is not clearly understood. A popular idea, already covered with relation to X100 line-pipe material in
chapter 3, is that of lattice matching, or misfit. Those inclusions having best lattice matching with the ferrite are most effective in nucleation. The uncontrollable nature of the quantity, distribution, size and structure of these inclusions contradicts this theory to some extent.

Ranking theory capable of determining the effectiveness of the various different kinds of non-metallic inclusions does not exist, though much evidence exists to identify titanium oxides \((\text{TiO}_x)\) to be potent, while alumina \((\text{Al}_2\text{O}_3)\) is not. Most welds contain a level of aluminium which in general is a stronger oxide former than titanium, these oxides of aluminium form first in the melt followed by \(\text{TiO}_x\) formations, normally seen to grow as thin coatings on alumina particles. It is therefore essential that sufficient oxygen is put into the system to first tie up the aluminium then combine with titanium. It is advantageous to minimise the aluminium content to the welding mix, as the oxygen content can then be reduced while still achieving the same titanium effect, and reducing the inclusion content. Any small amounts of aluminium that remains in solid solution, as opposed to forming oxide inclusions, causes the problem of promoting the formation of Widmanstätten ferrite, a nuisance when the desired microstructure is essentially acicular ferrite. Widmanstätten ferrite forms first leaving little residual austenite available for transformation to acicular ferrite.

The character of inclusions is seen to alter as the aluminium concentration rises, oxide particles being predominantly \(\text{MnO.SiO}_2\) at low concentrations. Raising the aluminium content changes the predominant oxide form to a mixed spinel oxide, galaxite, \((\text{Al}_2\text{O}_3\text{MnO})\) with further increase yielding alumina \((\text{Al}_2\text{O}_3)\). Common belief states that the aluminium to oxygen ratio should be such that the formation of galaxite is favoured, although for such multi-component systems containing strong de-oxidisers other than aluminium the ratio is difficult to determine as the soluble concentration of aluminium and other such elements cannot be calculated.

5.6.3 Improvement of the single output model

Through consideration of vital information acquired from previous modelling of acicular ferrite present in the weld metal it was decided that the single output model would be the approach developed further to improve results obtained. In an attempt to improve the performance of the single output model for acicular ferrite content of the weld metal, the number of inputs was reduced. Through the use of perceived significance results from the initial AF\% model, shown in
Figure 5.20 (a) and (b), input parameters carrying relatively low weightings could be identified for removal to form a new input architecture. Therefore, the following inputs were removed from the original single output architecture defined in section 5.6.1, forming a 13 input neural network architecture:

- Wire vertical stickout
- Weld wt.% Ni
- Spacing between wires 1 and 2
- Weld wt.% P
- Spacing between wires 2 and 3

Normalisation, randomisation and splitting were carried out as previously, yielding the same quantities of data for training, testing and validation. Results of error in the training and testing phase of the modelling process are shown in Figure 5.25, which are seen to be relatively lower than those of the initial AF% model containing 18 input parameters. Close examination of the error values gave no clear indication of the best neural network architecture because models with 7, 10 and 13 nodes in the hidden layer performed equally well when both training and test error were considered. After inspection of the predictions made across the training, test and validation data domains the 7 hidden unit architecture was found to be most robust. A comparison of the predictions made across the training, test and validation data domains for a neural network model for weld metal acicular ferrite content containing 7 hidden units can be found in Figure 5.26.
Figure 5.25 – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of weld metal acicular ferrite content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters.

Figure 5.26 – Comparison of predictions made using training, test and validation data for a neural network model for weld metal acicular ferrite content, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters.
Figure 5.27 (a) - Perceived significance, $\sigma_w$, for connections between input and output layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters.

Figure 5.27 (b) - Perceived significance, $\sigma_w$, for connections between input and hidden layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters.
Comparison of the predictions made across training, test and validation data domains, revealed that the error on predictions is far lower when compared with the 18 input model, therefore a higher level of confidence in predictions has been achieved. The improvement in the model is explained by the reduction in the number of modelling input parameters used. Examination of the perceived significance, $\sigma_w$, showed high weightings placed on weld metal wt.% O, wt.% Ti, wt.% Cr, plate thickness and welder travel speed. Perceived significance, $\sigma_w$, across the connections between input to output layer and input to hidden layer connections can be seen in Figure 5.27 (a) and (b) respectively, and further graphs of the weights on the connections can be found in appendix II, section 5. High weightings placed on the three alloying elements O, Ti and Cr are explained by the formation of inclusions within the weld metal, which are known to be strong nucleation sites for the formation of acicular ferrite. Examination of similar line pipe welds outlined in chapter 3, showed inclusions acting as potent acicular ferrite nucleation sites to contain high levels of titanium oxides. Plate thickness and welder travel speed are indicative factors to the thermal cycle produced during the welding process, although it is expected that if thermal cycle parameters play a strong role in the modelling that the heat input should play a larger role in the formation of the rules around the data.

5.6.4 Addition of weld bead area

The plate thickness and welder travel speed were seen to carry relatively high weighting upon the AF% model output, both being indicative of the weld thermal cycle, it was decided to add the weld bead area as an input in order to try and improve the predictive ability of the neural network. Inclusion of area mean the input architecture contained the following parameters; plate thickness, weld travel speed, measured heat input, weld metal wt.% C, Mn, Cr, Mo, Si, Al, Ti, S, N, O and weld bead area. Weld bead area is seen to be directly related to the cooling rate of the weld. As with all modelling, the more information required the less data becomes available to model with. Following the addition of weld bead area, and thorough pre-processing, only 133 data were available to the modelling process. The data were split into just training, 70 data, and testing, 63 data omitting a validation set. Modelling on this data was undertaken using a 14 input architecture and improvements were observed in the predictions made over the training and test data domains compared with previous modelling attempts. The error on training and testing, shown in Figure 5.28, was not found to be a smooth relationship decreasing with increased complexity of the neural network architecture and therefore an optimum model was not
determined in this way. Examination of the predictions made using training and test data revealed that a 10 hidden units model gave best results, and a graph showing actual points against predicted points for both training and test data domains can be seen in Figure 5.29.

![Graph showing average sum squared error with increasing complexity of neural network architecture](image)

**Figure 5.28** – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of weld metal acicular ferrite content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area

![Graph comparing predicted and actual AC%](image)

**Figure 5.29** – Comparison of predictions made using training, test and validation data for a neural network model for weld metal acicular ferrite content, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area
Figure 5.30 (a) - Perceived significance, $\sigma_{w}$, for connections between input and output layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area.

Perceived significance, $\sigma_{w}$, values, Figures 5.30 (a) and (b), revealed that across both input to output connections and input to hidden layer connections the rules formed weighted the weld metal Molybdenum (Mo) content far higher than any other input parameter. Molybdenum is added in carefully controlled amounts in order to influence the austenite to ferrite transformation, with the aim of obtaining a fine microstructure in the weld metal. Therefore, it would be expected to carry a relatively high weighting in the formation of acicular ferrite during the welding process, although the highly dominating nature of this input parameter might have a negative effect on the modelling. However, in order to evaluate the biasing of the network towards the wt.% Mo, the parameter was removed from the modelling data and the neural networks re-run using a 13 input architecture following the same pre-processing routine as with the 14 input model.
Figure 5.30 (b) - Perceived significance, $\sigma_w$, for connections between input and hidden layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area.

Errors from the training and testing phase with increasing complexity of the neural network architecture, once weld metal molybdenum content had been removed from the data, are shown in Figure 5.31, and can be seen to increase in comparison with the model that contained weld metal Molybdenum content. From the modelling of AF% using a 13 input architecture the optimum number of hidden nodes was found to be 10. This was not clear from examination of the error on training and testing, and further investigation was required taking into account predictions made across the training and testing data domains, shown in Figure 5.32. Comparing the predictions of the 13 input model with those made using a model containing Molybdenum weld metal content, as shown in figure 5.29, it is clear that the removal of this input parameter is detrimental to the performance of the model, and must therefore play a key role in the formation of the rules around the data.
Figure 5.31 – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of weld metal acicular ferrite content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area – wt.% Mo removed.

Figure 5.32 – Comparison of predictions made using training and test data for a neural network model for weld metal acicular ferrite content, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area – wt.% Mo removed.
The perceived significance values shed light on the role of other input parameters relative to one another, which were all small when weld metal molybdenum data was present. Perceived significance for the connections between input and output layer and input and hidden layer are presented in Figure 5.33 (a) and (b) respectively.

**Figure 5.33 (a) - Perceived significance, \( \sigma_w \), for connections between input and output layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area – wt.% Mo removed**
Figure 5.33 (b) - Perceived significance, $\sigma_w$, for connections between input and hidden layer, for a neural network modelling weld metal acicular ferrite content, containing 10 hidden units, using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area – wt.% Mo removed

Most interesting to note from the $\sigma_w$ results was the importance placed on the weld bead area directly related to the cooling rate of the weld in question. Formation of an acicular ferrite microstructure is dependent on the cooling rate of the welded area and the thermal cycle placed on the weld metal. However, results from predictions show the role of molybdenum cannot be ignored, Figure 5.34 highlights the distribution of data available for the normalised wt.% Mo compared with the plate thicknesses examined in these modelling trials; and similar graphs for all modelling data can be found in appendix II section 6. A good spread of data is found to exist for the weld metal Mo content, and therefore from the knowledge of the role of this key parameter in the welding process and the information as to the data distribution it is expected to play a significant role in the formation of acicular ferrite.
**Figure 5.34** – Distribution of weld metal Molybdenum content data compared with welded plate thickness for modelling data used in the network modelling of weld metal acicular ferrite content using weld metal chemistry and weld process parameters governing the thermal cycle as inputs described using a reduced number of input parameters and including weld bead area – wt.% Mo removed
5.7 Prediction of the occurrence of hydrogen induced cracking (HIC) in 3-wire single pass per side submerged arc welds using neural network modelling techniques

It is widely recognised that for the HIC failure to occur corrosion of the material must take place. The exact mechanism is not clear but popular theory suggests the accumulation of hydrogen at interfaces. Corrosion leads to the generation of atomic hydrogen atoms \((H^+)\), by the corrosion reaction of iron, usually combining to form hydrogen gas molecules, as outlined in equation 5.1. These hydrogen molecules either re-combine to form harmless hydrogen gas that bubbles off, or become absorbed by the steel. In the presence of sulphide or cyanide, the hydrogen recombination reaction is poisoned so that the atomic hydrogen atoms diffuse into the steel rather than recombining on the metal surface to form hydrogen gas.

\[
\begin{align*}
    \text{Fe} & \rightarrow \text{Fe}^{2+} + 2e \\
    2H^+ + 2e & \rightarrow 2\text{H absorbed} \\
    2\text{H absorbed} & \rightarrow \text{H}_2 \text{ (gas)} \\
    2\text{H absorbed} & \rightarrow 2\text{H absorbed}
\end{align*}
\]

The absorbed atomic form of hydrogen can diffuse through the ferrite matrix and become bound up at internal interfaces such as grain boundaries, inclusions or micro-phases. Given a sensitive microstructure and sufficient hydrogen concentration, the likelihood of hydrogen cracking occurring is high at a high enough tensile state in the structure. Hydrogen atoms that enter the pipeline can cause embrittlement and failure. It is interesting to note that usually HIC failures occur within a period of several days to a year of the pipeline being put in service.

5.7.1 Materials being investigated

A total of 219 welds manufactured using 1 pass-per-side 3 wire submerged arc welding, were HIC tested. The welds were manufactured using several plate sources, varying in thickness from 15.9 mm to 25.4 mm. Following welding the joins were either accelerated cooled or thermomechanically controlled rolled, giving equivalent strength levels varying between X52 and X65. Welding was carried out using OP122 agglomerated flux and 4 mm Ti-B and Ni-Mo alloyed wires. Heat input varied between 3.0 and 7.5 kJ/mm, with wire angles and spacing being varied for a given constant electrode stickout.
5.7.2 Inputs and output

Input parameters were initially defined prior to the pre-processing of the raw data. The inputs defined for the modelling of the occurrence of HIC were:

- Plate Thickness
- Welder Speed
- Measured Heat Input {Calculated from Wire Amps/Volts}
- Weld metal content:
  - Carbon (C)
  - Manganese (Mn)
  - Nickel (Ni)
  - Chromium (Cr)
  - Molybdenum (Mo)
  - Silicon (Si)
  - Oxygen (O)

A binary flag input was also used to identify the weld position as either inner diameter (ID) or outer diameter (OD). The output target is defined as a binary response, 1 standing for a HIC crack being present, and 0 for the weld being clear of any HIC damage. As the neural network model is dealing with a binary response from the data being presented to it, certain modelling parameters have to be altered to suit this type of data compared with the usual form of regression type modelling.

5.7.3 Binary response classification modelling

For a binary target it is possible to use a logistic regression model in which the probability of the target being "1" is obtained by passing the value of the output unit through the logistic function in equation 5.2:

\[ f(x) = \frac{1}{1 + e^{-x}} \]

The network, model, and data specification commands needed are quite similar to those used in the regression problem. Below are the command functions for a both a regression type model and a binary classification problem in Table 5.4 (a) and (b), which will be used to describe the difference in modelling technique being undertaken.
The 'net-spec' command here differs only in the number of input units (i) and the number of hidden units (h). The data model used is "binary", with no need for a noise level prior, as specified in the regression model. The 'data-spec' command for a binary model also states the inputs and outputs as found in a regression model. It also has a third argument of "2" just before the "/", which indicates that the target must be an integer with two possible values (which are "0" and "1").

# Commands to apply a Bayesian neural network to the simple regression problem.

net-spec work-?h-log.net i h o / - 0.05:0.5:1 0.1:0.5 - x0.1:0.5 0.05:0.5:1 1
model-spec work-?h-log.net real 0.05:0.5

data-spec work-?h-log.net i o / work.DAT@1:300 . work.DAT@301:600 .

net-gen work-?h-log.net fix 0.5
mc-spec work-?h-log.net repeat 10 sample-noise heatbath hybrid 100:10 0.2
net-mc work-?h-log.net 1

mc-spec work-?h-log.net sample-sigmas heatbath hybrid 1000:10 0.4
net-mc work-?h-log.net 1000

Table 5.4(a) – Command line functions for a Bayesian neural network applied to a simple regression problem.

The initial phase commands that were used for the simple regression problem {net-gen, mc-spec and net-mc} turn out to be adequate for this problem as well; sample-noise operation statements are actually unnecessary, since there is no noise for this model. Sampling phases use commands similar to those in the regression modelling, but the changes presented in the binary data model give better results and faster convergence. It is worth noting that the mc-spec command needed here is long, so it is continued by putting a "\" at the end of the first line.

The last 'mc-spec' command specifies the variant of hybrid Monte Carlo utilised along with "persistence", in which relatively short trajectories are used but random walks are suppressed by only partially replacing the momentum in the 'heatbath' step. Note that for this to work well, the
rejection rate must be quite small. This alternative method has the advantage that it allows for more frequent hyperparameter updates using 'sample-sigmas'.

# Commands to apply a Bayesian neural network to a problem with a binary response.

net-spec HIC-?h-log.net i h o / - 0.05:0.5:1 0.1:0.5 - x0.1:0.5 0.05:0.5:1 l
model-spec HIC-?h-log.net binary

data-spec HIC-?h-log.net i o 2 / HIC.DAT@l:x . HIC.DAT@x+1:n .

net-gen HIC-?h-log.net fix 0.5
mc-spec HIC-?h-log.net repeat 10 sample-noise heatbath hybrid 100:10 0.2
net-mc HIC-?h-log.net 1

mc-spec HIC-?h-log.net sample-sigmas heatbath 0.95 hybrid 100:10 / 0.3 negate
net-mc HIC-?h-log.net 1000

---

Table 5.4(b) – Command line functions for a Bayesian neural network applied to a problem with a binary response.

5.7.4 Results of neural network modelling of the occurrence of HIC from welding parameters and weld metal chemistry

Initial testing was carried out on all data available for HIC evaluation; a total of 219 welds were considered, of these welds 21 were found to have HIC damage the remaining 198 were classed as being clear. These data were normalised using the method outlined below, in equation 5.3, scaling the data to have zero mean and standard deviation equal to 1, unlike the favoured scaling between -0.5 to 0.5 for regression type modelling. The use of this normalisation was due to the binary classification working at the extremes of the activation function; therefore normalisation to the limits suits the problem much better.

\[ x_{i,\text{norm}} = \left( \frac{x_i - \bar{x}}{\text{std}} \right)^{\text{nstd}} \]  

5.3
\( x_i \) identifies each value of the specific input or output column, \( \bar{x} \) is the mean of the data in that column. The standard deviation (std) of the raw data is defined in equation 5.4 below, and \( \text{nstd} \) is defined as the new standard deviation of the normalised data usually assumed to equal 1.

\[
\text{std} = \frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N-1}
\]

Normalised data were randomised and run using a binary response network, using 1000 Markov chain Monte Carlo steps. The ratio of HIC positive data to HIC negative data caused obvious problems with the neural network; biasing the data and generalisations made by the neural network model. Observations of the predictions made using all the data showed that the network generalised on the clear samples and therefore all predictions indicated that whatever the input the output indicated a "clear" weld.

5.7.5 Balancing the data

Extracting the relevant data for the 21 HIC welds which did crack, and randomly selecting data for 21 welds that were classed as clear allowed the formation of a more balanced data set. The same inputs to outputs were used, splitting the total of 42 data to give 21 training data and 21 testing data. Balancing the ratio of HIC positive to HIC negative target values evened out the bias on the data and results were good, showing 95% accuracy over the domain represented by the training data. Figure 5.35 shows the average sum squared error across the program of modelling considering the effect of increasing the number of hidden units in the network architecture. From this it is found that 7 hidden units carry the most accurate modelling capabilities, although a 2 hidden unit model will re-produce similar results but the level of confidence is lower.

The selection of random HIC clear welds was repeated to examine the robustness of this technique, and the results showed again that HIC occurrence could be predicted to within 95% accuracy. It was interesting to note that upon examination of the model containing just one hidden unit (basically a linear regression model) the first model showed 95% accuracy whereas
the second attempt showed only 52% accuracy. An explanation for this change in performance is that the HIC clear welds in the 1st attempt were grouped much closer together than those in the second attempt. HIC clear data in the second model covered a far greater range of welds, and is a far better approach to selecting data for this modelling exercise.

Figure 5.35 — Average sum squared error against the complexity of the neural network model for HIC occurrence modelling using welding parameters and weld metal chemistry from a reduced data set (42 data)

The graph in Figure 5.35, illustrates that the 1 hidden unit neural network architecture yields relatively poor training and test errors when compared to more complex modelling architectures, although the benefits of a neural network model containing more than 2 hidden units are minimal. Predictions made during the testing phase can be examined using the command, "net-pred itmp xxxxx-log.net 300:," these results are displayed in Table 5.5 outlining the normalised inputs and the predicted outcome against actual outcome.
5.7.6 Evaluation through examination of input relevance

In order to evaluate the level of confidence in predictive capabilities of the neural network model, the perceived significance, $\sigma_w$, of inputs and weights on connections between the input, output and hidden layer were examined. Figures 5.36 (a), (b) and (c) show results of the inspections of weights across the connections in the input, hidden and output layers. Weights across the connections between input and output layer are shown in Figure 5.36 (a), the average of the weights across the connections between inputs and the hidden layer for each input parameter are considered in Figure 5.36 (b) while Figure 5.36 (c) shows the mapping of the weight space between input layer and hidden layer. As is seen from Figure 5.36 (a), plate thickness and weld travel speed carry the largest influence through the input to output, with all other inputs carrying relatively little weighting. As the plate thickness and welder travel speed are indicative of the weld metal heat input and cooling, and the diffusion of the hydrogen being dependent upon specific temperature ranges, these would fall out of the equation as the linear type inputs.

More complex influence issues as regards the mapping of data between inputs to output can be found through investigation of the weighting across the connections between input nodes to hidden nodes. Due to the large number of inter-connections between input layer and hidden layer, a large amount of information is retrieved. In order to summarise this information, an average for each input across the range of hidden nodes is taken, as shown in figure 5.36 (b). As the weightings can be either negative or positive this can sometimes be misleading, therefore it is better to consider a map of these weights across the complete weight space in order to identify strong or weak positive and negative values shown in Figure 5.36 (c).
Number of iterations used: 701

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Average log probability of targets: -0.403

Fraction of guesses that were wrong: 0.0476 +/- 0.0476

Table 5.5 - Results for a neural network predicting a binary response for the occurrence of HIC, taken from testing phase
Figure 5.36 (a) – Weights on connections between input and output layer for a binary response neural network model for HIC occurrence

Figure 5.36 (b) – Average weights for connections between input and hidden layer for each individual input for a binary response neural network model for HIC occurrence
Figure 5.36 (c) – Weight map for connections between input and hidden layer for a binary response neural network model for HIC occurrence. Inputs – (1) ID/OD Run, (2) Plate Thickness, (3) Welder Travel Speed, (4) Heat Input, (5) Weld wt.% C (6) Weld wt.% Mn (7) Weld wt.% Cr (8) Weld wt.% Mo (9) Weld wt.% Si (10) Weld wt.% Ni (11) Weld wt.% O

Examination of the information gained in the graphs in figure 5.36 (b) and (c) shows that there is far more interaction from all inputs passing through the hidden layer than those connecting directly from input to output layer. Figure 5.36 (b) highlights the increased relative influence of the chemical elements namely weld wt.% Cr and weld wt.% O. The welder travel speed and plate thickness also figure highly and are responsible for the high temperature heat cycle taking place. Comparing these results with the mapping for the weights across the input to hidden connection space in figure 5.36 (c), the two biggest influencing factors are welder speed and weld metal chromium (Cr) content.

5.7.7 Discussion of the Results of the HIC Classification Model

Due to the hazardous means of testing HIC crack occurrence in weld metal, collection of data is a costly and time consuming task. Examination of the modelling data identifies only 10% of available welds showing any positive signs of HIC failure. Establishing a suitably sized database for accurate modelling of HIC across a wide range of weld chemistries and welding parameters would be an extremely difficult task. The necessity for the database to carry an even balance of
positive and negative results makes the task yet more difficult. This work considers a small amount of data, modelling the range of welds manufactured to the best possible standard considering data constraints used in training and testing of the neural network model.

Results of the testing phase highlight the confidence in predicting the occurrence of HIC to be at 95%, this is relatively high in comparison with linear regression models. As the data provided to the network was evenly balanced and the output taking a binary form this would be expected from a well trained neural network model. Investigation of the input relevance has shown that the input parameters with highest influence are; plate thickness, welder speed, heat input and weld metal wt.% Cr and O.

Chromium is influential in the transformation of austenite to ferrite during the solidification of the weld metal along with other elements including manganese and molybdenum; HIC is found to be more likely to occur in ferritic or martensitic structures. Chromium has also been found to be one of the elements giving a substantial reduction in absorbed hydrogen\(^ {119, 120}\). Chromium carries a high negative weighting across the connection space between input and hidden layer, this relates directly to the fact that increasing Cr content would lead to a decrease in the chance of HIC occurrence. To a lesser extent weightings on Mn and Mo are observed, although higher weightings might be expected here. Examination of the data used showed no biasing towards Chromium data patterns relative to the HIC data, when compared with the data used for Mn and Mo content of the welds. A far greater spread of data is present in this small data set for the content of Mo and Mn compared with Cr content as seen in Figure 5.37, this is attributable to the high weighting placed on the Cr content.
Figure 5.37 – Spread of data for wt.% Cr, Mn and Mo used in training a neural network model to predict the presence of HIC cracking in weld metal

The weighting placed on weld wt.% O is explained by the fact that hydrogen becomes bound at interfaces such as inclusions, with inclusions normally being oxides of other alloying additions, or oxidised impurities present in the parent plate from the plate forming process. In the manufacture of X65 line pipe these inclusions are mainly in the form of Al₂O₃ (alumina), TiO (titanium oxide), and smaller quantities of MnO·SiO₂ (rhodonite), with other nitrides, sulphides and carbides also being present dependent on the alloying mixture being input to the welding process. Where moderate aluminium content is present a spinel known as galaxite (MnO·Al₂O₃) is formed usually in the place of alumina. Large alumina particles in addition to manganese sulphide were found to be present on HIC fracture surfaces in the work of Brown and Jones¹²¹. In conclusion, an increase in the oxygen content of the weld metal will lead to an increase in oxides being found in the form of inclusions, these inclusions being a major contributor to entrapment of hydrogen and initiators for cracking in HIC failure.
5.8 Conclusions

- An attempt to predict weld metal composition using neural networks has been made, following on from previous work and using the findings to produce the best models using a 5 input architecture. Normalising between the limits -0.5 and 0.5 was found to yield better results than using data normalised to give zero mean and standard deviation equal to 1. For most of the elements a good neural network model is obtained using few hidden units.

- Simple neural network models considering plate and wire chemistry for a particular element are, in general, not significantly better than other existing methods such as multiple linear regression, probably because there is an intrinsically simple physical relationship between weld, wire and plate chemical compositions. It has become apparent that there is a lower limit to the amount of data that can be used to accurately model data using neural network. This limit is dependent upon the broadness of the distribution of the data.

- Improvements to the neural network modelling of weld metal chemistry has been identified through the use of a multiple output model. This model gains an advantage because it is able to consider data regarding input chemistry for all modelled chemical elements, and the eventual chemical analysis for each modelled chemical element in the weld metal, thus taking into account the information required to consider the complex chemical reactions that take place in the weld pool.

- A regression type model has been developed to predict the weld metal acicular ferrite content to a high level of confidence, taking into account important alloying elements and parameters influential to the weld thermal cycle.

- Multiple output models with a primary aim of predicting acicular ferrite, while also considering primary ferrite and ferrite side plate, do not carry an advantage over a singular output acicular ferrite model for the types of welds being considered. This is a result of the weld being in excess of 90% acicular ferrite content.

- A binary response model has been developed to predict the occurrence of HIC cracks in weld metal, given weld metal chemistry and basic welding parameters as inputs. This model is
highly accurate within the range of the data domain for which it is trained. Training of binary response models requires a good balance between positive (1) and negative (0) response training patterns. A shift in this balance causes a shift in the responsive nature of the model, in the direction in the shift in balance of the data.
5.9 Chapter Summary

Initial modelling exercises have been covered in this chapter considering some simple relationships, and then these neural network strategies have been developed to investigate more complex data patterns, whilst improving the predictive capabilities for the desired target outputs. Modelling in this chapter has considered regression type relationships used in the neural network modelling of weld metal chemistry and microstructure, and binary classification modelling occurrence of HIC failure in steel line-pipe welds.

Modelling of weld metal chemistry is shown to yield good results by considering the simple relationship between plate and wire chemistry compared with the chemistry of the weld metal. Modelling simple relationships does not truly exploit the usefulness of neural networks in finding patterns within the data examined; comparisons with linear regression techniques highlight this fact. In an attempt to improve on this initial work a multiple output neural network model evolved which employed the plate and wire chemical content of all weld metal elements found in the output layer, as input variables. This use of a multiple output modelling greatly exploits the data mining abilities of neural networks, especially for those elements predicted badly (e.g. oxygen and phosphorus) using single output modelling.

Moving on from the modelling of weld metal chemistry, weld metal microstructure was considered with the idea that the chemistry model outputs are to be fed forward to the input layer of a model for the weld metal microstructure. This work considered a single output model for acicular ferrite and a three output model for acicular ferrite, primary ferrite and ferrite side-plate; the three major microstructural constituents in the welds modelled. Both modelling approaches considered chemistry and welding parameters influential in the thermal cycle experienced by the weld metal. It was found that using a single output for acicular ferrite produced the best results, which was not surprising as the welds considered were over 90% acicular ferrite microstructure content, with not much distribution in the data for other microstructure constituents.

The occurrence of hydrogen induced cracking (HIC), though not strictly a chemical or microstructural characteristic, was included with this work firstly a means of demonstrating the ability to interpret data using binary classification models in contrast to the more precise regression style modelling, and secondly as the modelling techniques considered parameters in a
similar vein to those of the chemistry and microstructure modelling. Results of this modelling show a good correlation between actual and predicted results, with a 95% level of accuracy, although due to the small number of data used in training and testing the neural networks the predictions are only good for the small data domain used. This lack of data stems from the costly and time consuming method whereby HIC testing results are obtained, testing for the sensitivity of an alloy to HIC failure, and therefore it is expected that a small number of positive HIC results are found.

The techniques in this chapter highlight the type of models that can be undertaken through the use of neural networks to a high level of confidence, and will be applied to more complex and novel approaches. The areas of welding that will be considered in later chapters are weld metal mechanical properties and weld geometry, previously not approached in any depth from first principles due to the complex relationships between manufacturing parameters and end result.
Chapter 6 - Prediction of multi-wire submerged arc weld bead shape using neural network modelling techniques

6.1 Introduction

The manufacture of large diameter line-pipe involves the forming of plate to pipe, seam welding, followed by expansion of the pipe to final shape as discussed in chapter 2. The weld may thus be viewed as part of an overall process involving the pre-forming and post-forming operations. This type of manufacturing route lends itself to through process modelling where the challenge is to develop algorithms for different parts of the production process and link these to form on-line or off-line models.

The seam welding operation in the manufacture of large diameter line-pipe is generally carried out using the high productivity, multi-wire, submerged arc welding (SAW) process, involving one pass per side welds. Bead shape, size, alignment and interpenetration are important in terms of weld quality, as also are the amount of residual stress and distortion, although ultimately the quality of the weldment is defined in terms of mechanical properties such as strength and toughness. In deciding the welding procedure to achieve a given set of properties, the welding engineer tends to choose welding parameters on the basis of prior experience, but a number of experimental trials may be carried out, particularly for new projects, eventually leading to a definition of the optimal welding parameters. This process is often time consuming and expensive. A more flexible and rigorous approach would be to develop algorithms to predict the required properties from process parameters and link these into a through process model.

There are many factors affecting the final weld properties including weld metal and parent plate chemical composition, section thickness, number of weld passes and heat input. The heat transfer from a weld to its surroundings is particularly important. Welding parameters, determine the amount of re-heated parent plate and, in the case of multipass welds, the previously deposited weld metal. The ability to predict the thermal history at any point in the weld surroundings is an important step to modelling weldment residual stress, distortion, microstructure and properties.

In large diameter linepipe seam welding, the weld beads may vary significantly in size and shape depending on pipe wall thickness. For small section linepipe (less than ~15mm), the beads may
be small and round in shape whereas, at large section sizes, the beads may be narrow and deeply penetrating. The beads may also be flared towards the surface of the plate and the weld cap may approach the plate surface at an acute angle. Heat flow in line-pipe seam welds, is therefore complex. In order to predict accurately the thermal history at a point in the weld bead surroundings, it would appear important to develop a capability to model complex weld bead shapes. This then has the potential to be further linked to models for heat flow, strain and distortion, or be used as a basis for the theoretical modelling of multipass weldment microstructure and properties to produce complete through-process models.

Many theories and models have been put forward as to the effect of varying process parameters on the eventual bead shape for different types of welding. Even though physical models based on fundamental equations have become increasingly sophisticated and can account for several of the mechanisms that influence weld shape, they are still not useful for most production applications. These models usually require substantial computer processing power, and are often far too slow for real time simulations. More recent models have made use of neural network techniques enabling prediction of situations too complex for simple analytical models or multiple linear regression techniques.

6.2 Modelling Methodology

With any numerical modelling process a quantitative method of representing the inputs and outputs is always required, this section highlights the novel methods used in capturing the weld bead shape in a workable form for the modelling undertaken. Methods for measuring covering scaling, accurate measurement and consistent positioning of the origin are covered for transformation of the weld bead shape to a numerical form. The chapter also covers the data used highlighting the reasons behind the methods developed towards predictions of weld bead shape.

6.2.1 Weld Data

The data used in this work contained information for welds manufactured under experimental conditions using 3 wire submerged arc welding with one pass per side, comprising single outer diameter (OD) and inner diameter (ID) beads, which were either balanced or unbalanced. A balanced weld is defined as one in which the OD and ID beads are of similar size, and an unbalanced weld as one in which the OD bead is substantially larger than the ID bead. It should
be noted that all of the welds were manufactured using a tack weld, either continuous or intermittent, initially placed in the preparation for the OD bead, prior to deposition of the ID bead, and subsequently the OD bead. The welding parameters, and plate and wire chemistries, were typical of those used in line-pipe seam welding. The plates welded ranged in thickness from 15.9 to 25.4 mm, and were either accelerated cooled or thermo-mechanically controlled rolled. The plates were alloyed with either Nb or Nb and V, and varied in strength from X52 to X65. Welding was mainly carried out using 4 mm diameter wires alloyed with Ti-B or Ni-Mo, together with Oerlikon OP122 agglomerated flux. Heat inputs varied between approximately 3.0 and 7.5 kJ mm\(^{-1}\), with DC applied to the lead wire, and AC on the remaining two. Different wire angles (30-60°) and spacing were used, with an electrode stick out between 35 and 45 mm. An overview of the range of data available can be seen in Table 6.1. In total weld macrostructures and process data were available for 164 different experimental conditions.

6.2.2 Digitisation of weld macrostructures

Weld macrographs were taken using a 35mm camera with Ilford FP4 Plus black and white film, and digital images produced from the negatives were subsequently used for measurement. A polar coordinate system was used in order to limit the amount of data needed to represent the weld bead shape for the neural network, with a constant angular measurement for all welds, the variable being the distance from the origin at each angle. Care was taken to set the origin for all welds in order to obtain consistency during measuring. The x plane was taken to be in line with the points of contact between the weld bead and plate surface and a parallel line drawn to form a tangent with the deepest point of the weld. These two lines were then used to position a measuring grid; the grid consisting of lines from an origin at equally spaced angles. The exact x axis position was determined by rotation to fit with the points of contact between the weld bead and plate surface, and the y axis was positioned at 90° to the point of the tangent with the deepest point of the weld, as shown in Figure 1. However, in order to take accurate measurements the image was initially measured using an x-y co-ordinate system on a suitable computer package, which enabled the image to be enlarged easily, allowing better determination of the edge of the weld and beginning of the HAZ. These x-y co-ordinates were then translated to a polar co-ordinate system for use as input data in the neural network. Scaling of the image was determined by taking a diagonal measurement on the image from the point of contact of the OD bead and the plate surface, and the opposite point of contact of the ID bead and the inner plate surface. This was used in conjunction with a measurement of the actual weld carried out using a digital
calliper, to give a scaling factor. Measurements were typically taken every 15° between 0 and 345°, with additional measurements at 82.5°, 97.5°, 262.5° and 277.5° being used to ensure that the bay area of the weld bead was accurately taken into account.

<table>
<thead>
<tr>
<th></th>
<th>Plate Thickness (mm)</th>
<th>Prep Angle (°)</th>
<th>Prep Depth (mm)</th>
<th>AMPS Wire1 (A)</th>
<th>VOLTS Wire1 (V)</th>
<th>ANGLE Wire1 (°)</th>
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</thead>
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<table>
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<th>VOLTS Wire2 (V)</th>
<th>ANGLE Wire2 (°)</th>
<th>AMPS Wire3 (A)</th>
<th>VOLTS Wire3 (V)</th>
<th>ANGLE Wire3 (°)</th>
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</thead>
<tbody>
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<td>7.5000</td>
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<td>46.0000</td>
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<td>645.0000</td>
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<td>36.8150</td>
<td>3.7900</td>
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<td>42.3950</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>Welder SPEED (mm min⁻¹)</th>
<th>STICKOUT (mm)</th>
<th>SPACE 1_2 (mm)</th>
<th>SPACE 2_3 (mm)</th>
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</thead>
<tbody>
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<td>45.0000</td>
<td>21.0000</td>
<td>23.0000</td>
</tr>
<tr>
<td>Min</td>
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<td>35.0000</td>
<td>19.0000</td>
<td>19.0000</td>
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<tr>
<td>Average</td>
<td>1326.1000</td>
<td>42.4300</td>
<td>19.6500</td>
<td>20.0300</td>
</tr>
</tbody>
</table>

Table 6.1 - Statistics on the process parameters used for the welds considered in modelling.

6.2.3 Data Pre-Processing

The process data and measurements were normalised before being input into the neural network in order to eliminate any biasing that may occur due to differences in magnitude of the values being used as inputs and outputs. The scaling applied in the normalisation phase is then reapplied to predictions made by a fully trained network, to produce actual values. There are a number of ways in which to normalise the data and it should make no difference which method is used. In this case the data were scaled between -0.5 and +0.5, according to the formula in equation 4.6.
The next step was to randomise the data, and split the data into a training and test data set to ensure that both the training and test data were representative of the system as a whole. In this case, due to the relatively small amount of data available, all 164 data were used in the training and testing of the neural network, with 82 training data used to form a model, and 82 test data to predict values of the output. It should be noted that in order to create a validation set, the data are un-shuffled and re-combined before being fed into the best neural network architecture.

6.2.4 Pictorial representation of the weld bead shape

In order to compare qualitatively the predicted and actual weld bead shape, images were drawn using a simple 2D CAD package. The image was constructed using the predicted output of polar coordinates, angle and bead shape extent, from the neural network. It should be noted that the number of predicted outputs limits the number of measurements used in creating the geometry of the predicted weld bead. In an effort to represent the actual weld bead as accurately as possible 28 measurements were used.

Due to the nature of the software and the measuring method used in describing the weld bead shape, a level of interpolation is present in these images when a curve is drawn to fit the input measurements. The greater the number of points used in describing the shape to be drawn, the lower the amount of interpolation between points. It was decided, in order to avoid excessive interpolation, especially in the region where the weld cap meets the parent plate, to draw the bead shape using two separate curves. These two curves both have their ends at the 90° and 270° positions (see for example Figure 6.1), hence ensuring that the extent of the weld bead is represented pictorially in such a way as to reflect the predictions made by the neural network model.
Figure 6.1 - Selection of origin and positioning of the measuring grid on the OD weld for a typical one pass per side 3 wire submerged arc weld.

6.2.5 Input Relevance

A useful tool when evaluating the confidence in the predictions made by a neural network, is to consider the weighting placed on the various inputs used by the neural network model, better known as input relevance. Input relevance can be accessed in a variety of ways\textsuperscript{124}, including the use of artificial data, and also through information stored within the neural network architecture.

By performing simple ‘thought’ experiments that investigate variation in one input variable whilst keeping the others constant, the influence of the chosen input can be investigated quantitatively. As the inputs are normalised it is possible to compare equal relative changes. An example is to feed into the neural network two data sets created when all the inputs are set to zero and one of them set to the value 0.25, and similarly with all set to zero and one to -0.25. It is obviously necessary that in order to use this method, all the inputs must be continuous. Also it is important to note that this combination of values selected by hand does not represent a real experiment, rather a ‘thought’ experiment that throws light on the relevance of each of the inputs.

It is also possible to closely examine the neural network architecture in order to evaluate the weighting placed on the connections between the various nodes in the different layers of the
neural network model. An extensive amount of potentially overwhelming information is available, especially for large and complex network architectures. In order to extract the relevance placed on individual inputs, it is possible to examine the hyperparameters, or sigma values, between the different layers\textsuperscript{53}. A hyperparameter can be thought of as being an additional value associated with every parameter in the network. In this work, sigma values for connections between the input and output layers have been used to determine the influence of changes in each input on the output, i.e. weld bead shape. Values were also determined for the sigma values between the input and hidden layer, and the hidden layer and output layer separately. However, these values were found to reveal no additional information compared to that between the input and output layers directly.

The different areas of the weld bead shape are influenced by different welding parameters, and therefore it is useful to explore the neural network model by considering the input relevance separately at the 0°, 90°, 180° and 270° relative positions.

6.3 Initial Model

12 points were first used to describe the geometry of the weld bead by using measurements taken at 30° intervals around the grid. These were used in the initial modelling concept to construct a network architecture consisting of 16 inputs involving the welding parameters, see Table 6.2, and 12 outputs, each being the extent of the weld bead as a function of position. The number of hidden units was changed in order to optimise and evaluate the neural network model. This work considers the full 164 data sets available for the modelling of weld bead shape, though proof of concept was carried out using just 100 of the data. This number of data was found to be insufficient, yielding results with a low level of confidence in prediction, therefore the higher number of data were introduced.
6.3.1 Results of Initial Modelling

![Graph showing the average sum squared error, compared with the increased complexity of the neural network architecture, considering the bead shape as a whole.](image)

Figure 6.2 - Graph showing the average sum squared error, compared with the increased complexity of the neural network architecture, considering the bead shape as a whole.

Figure 6.2 shows that with improving training error, there is a definite rise in the test error, which suggests that over-fitting is present. This is where the neural network is using a much too complicated relationship between inputs and outputs, therefore the generalisation used in making predictions is poor. In this case, the test error was a summation of all the 12 outputs (positions) considered, and therefore was artificially higher than if the neural network were trained with each measured output individually. Nevertheless, predictions were made using this model, taking the best neural network architecture to contain 12 hidden units, as there is a fall in the test error without any related peak forming in the training error, which was at an acceptable level.

In order to investigate the quality of predictions produced by the various neural network models, 6 particular weld beads from the dataset were chosen which varied widely in size of weld bead, depth of penetration and symmetry of the weld bead. The predicted shapes of the weld beads are compared with the observed shapes in Figures 6.3 (a-f), together with a graph plotting actual data for the particular weld bead against predicted data. The ideal case would be for the plot to fit along the ‘y = x’ line, which would give two images overlaying one another exactly. There is some variability in the six examples as to the quality of bead shape predictions, probably due to the over-fitting found to have occurred in the training of the neural network. All of the predictions made, using the 164 data sets, have been plotted against the actual measurements...
taken in Figure 6.4. These predictions were undertaken on both a neural network model containing just one hidden unit (Figure 6.4a), which can be assumed to be equivalent to a linear model, and on the chosen architecture of 12 hidden units (Figure 6.4b) used in the predictions in Figure 6.3. It is clear that the use of a neural network architecture has improved the confidence with which predictions can be made, with far more points fitting to the ‘$y = x$’ line.

<table>
<thead>
<tr>
<th>Input</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amps1</td>
<td>Current at each respective wire</td>
</tr>
<tr>
<td>Amps2</td>
<td></td>
</tr>
<tr>
<td>Amps3</td>
<td></td>
</tr>
<tr>
<td>Volts1</td>
<td>Voltage at each respective wire</td>
</tr>
<tr>
<td>Volts2</td>
<td></td>
</tr>
<tr>
<td>Volts3</td>
<td></td>
</tr>
<tr>
<td>Angle1</td>
<td>Angle of each respective wire from vertical</td>
</tr>
<tr>
<td>Angle2</td>
<td></td>
</tr>
<tr>
<td>Angle3</td>
<td></td>
</tr>
<tr>
<td>Space12</td>
<td>Spacing between wires</td>
</tr>
<tr>
<td>Space23</td>
<td></td>
</tr>
<tr>
<td>Speed</td>
<td>Travel speed</td>
</tr>
<tr>
<td>Stickout</td>
<td>Wire vertical stickout</td>
</tr>
<tr>
<td>Thickness</td>
<td>Plate thickness</td>
</tr>
<tr>
<td>Prep_Angle</td>
<td>Weld v-preparation angle</td>
</tr>
<tr>
<td>Prep_Depth</td>
<td>Weld v-preparation depth</td>
</tr>
</tbody>
</table>

**Table 6.2** - The inputs and outputs used in the construction of the neural network model architectures.
Prediction of Multi-wire submerged arc weld bead shape using neural network modelling techniques

(a)

(b)

(c)
Figure 6.3 - Comparison of the actual (solid line) and predicted (dashed line) images for the initial neural network model, considering the bead shape as a whole, along with the actual measured data plotted against predicted data for each individual predicted image.
6.3.2 Initial Model – Input Relevance

Input relevance testing was carried out on the neural network model using the two methods described above. Figure 6.5 illustrates the sigma values determined for the relationship between the inputs and outputs directly. It can be seen that preparation depth is predicted to be the most influential, with current on the lead wire, and volts on the second wire also having a role to play. It is interesting to note that the preparation angle is not predicted to have any significant influence on the weld bead shape with the preparation depth being the major dominating factor. Few other weld process variables show any substantial effect on the predictions made of the weld bead shape compared with those mentioned above; plate thickness, speed, electrode stickout and spacing being of comparable, but much smaller, importance.

Figure 6.4 - Comparison of actual data against predictions for a linear model (a), and the chosen neural network architecture with 12 hidden units (b), for the neural network model considering weld bead shape as a whole.
The results of the input relevance tests performed at the 0°, 90°, 180° and 270° positions are presented in Figure 6.6 for the initial modelling architecture considering the weld bead shape as a whole. The output is the extent of the weld bead at each of the four angles, and the bar height represents the influence of setting a particular input variable to its maximum or minimum value, whilst keeping all other values at zero. It can be seen that preparation depth plays a major part in all areas of the weld, this being the determining factor as to where the volume of molten weld metal is deposited. It should also be noted that increasing the preparation depth results in the prediction of a deeper weld, with a shallower cap, as expected. It is also interesting to note the influence of the welding speed at the 90° and 270° positions, i.e. at the extent of spread of the weld bead.

From the initial model, it can be seen that weld bead shape can be predicted to a relatively high level of confidence. However, there is some variability due to the complex nature of the relationship between the inputs and outputs and the high number of points predicted from one
model. There is, however, a definite improvement in the confidence with which prediction of bead shape can be undertaken using a neural network approach from process parameters when compared with a linear model.

![Graphs showing input relevance performed on the 12 hidden unit neural network architecture considering the bead shape as a whole, evaluating predictions at different angles.](image)

Figure 6.6 - Input relevance performed on the 12 hidden unit neural network architecture considering the bead shape as a whole, evaluating predictions at (a) 0° (b) 90° (c) 180° and (d) 270°.

### 6.4 Development of the Model

The number of points used in describing the geometry of the weld bead appears to affect the accuracy of the predictions made overall due to the balance between the number of inputs and datasets used. However, using a larger number of points results in a better representation of the weld bead in specific cases, especially where there is the occurrence of a bay area. With the need to limit the number of target outputs, a possible solution is to split the weld bead into
distinctive areas, and create a number of different neural network models to predict the bead shape. To ensure continuity between each neural network model, it was decided that the areas modelled should either share a boundary or have overlapping boundaries. It was also decided to include the area of each modelled region as a controlling parameter in order to constrain the prediction of lengths as a function of angle. The area of the weld bead shape was calculated using the summation of areas from individual triangles, using the measurements of each of the two sides and the included angle.

6.4.1 Boundary Model

It was decided to split the whole weld bead into four separate areas, essentially containing the cap, the bottom and two sides of the weld bead. The inputs used were the same as those for the single model of the whole weld bead, the differences being in the number of target outputs. Area A, the cap, contained output lengths measured at 285, 300, 330, 0, 30, 60 and 75°; area B, the right hand side at 75, 90, 120 and 135°; area C, the lower part of the weld bead, 135, 150, 180, 210 and 225° and area D at the left hand side, 225, 240, 270 and 285°, as shown in Figure 6.7.

![Figure 6.7](image-url)

**Figure 6.7** - A schematic diagram illustrating the four areas used in the development of the boundary model.
Neural network models were trained, tested and evaluated as a function of the number of nodes in the hidden layer as previously. Figure 6.8 presents a graph of the average sum squared error against increased complexity for the four models in each area. It can be seen once again that the training error in all four models is acceptable, although there is a varied response from the testing errors, with the worst level of test error resulting from the model for area A, the weld cap area. The optimum number of hidden nodes in each neural network varied, depending on the area being considered with 9 hidden units being chosen for areas A and C, 7 for area B and 11 for area D.

Figure 6.8 - The average sum squared error as a function of the number of hidden units for the four neural network models, areas A (0°) – D (270°C), for the boundary model.

It is clear from the images in Figure 6.9, for the same weld beads as those discussed in Figure 6.3, that there is a problem with continuity between models when they meet each other at a boundary. Such boundary points are also being predicted in two neural network models for the adjacent areas, and therefore this begs the question as to which should be used in the representation of the image. Therefore, in order to overcome this problem it was proposed instead to use an overlapping boundary model.
Prediction of Multi-wire submerged arc weld bead shape using neural network modelling techniques

(a)

(b)

(c)
Figure 6.9 - Comparison of the actual (solid line) and predicted (dashed line) images for the boundary neural network model, along with the actual measured data plotted against predicted data for each individual predicted image.
6.4.2 Overlapping Boundary Model

It was again decided to split the whole weld bead into four separate areas, essentially containing the cap, the bottom and two sides of the weld bead. The inputs used were the same as those for the single model of the whole weld bead, the differences being in the number of target outputs. Area A, the cap, contained output lengths measured at 300, 330, 0, 30 and 60; area B, the right hand side at 30, 60, 90, 120 and 150°; area C, the lower part of the weld bead, 120, 150, 180, 210 and 240° and area D at the left hand side, 210, 240, 270, 300 and 330°, as shown in Figure 10. It should be noted that a slightly reduced number of target outputs were considered in this case to investigate whether an overlapping boundary makes an improvement on previous predictions.

Figure 6.10 - A schematic diagram illustrating the four areas used in the development of the overlapping boundary model.

Neural network models were trained, tested and evaluated as a function of the number of nodes in the hidden layer as previously. Figure 6.11 presents a graph of the average sum squared error against increased complexity for the four models in each chosen area. It can be seen once again that the training error in all four models is acceptable, although there is a varied response from the testing errors, with the worst level of test error once again resulting from the model for area A, the weld cap area. This graph provides an indication that the neural network models include a degree of over fitting, in that the training error is generally low with an increasing test error. The
optimum number of hidden nodes in each neural network varied, depending on the area being considered with in this case 11 hidden units chosen for areas A and D, 12 for area B and 10 for area C.

Figure 6.11 - The average sum squared error as a function of the number of hidden units for the four neural network models, areas A (0°) – D (270°), for the overlapping boundary model.

The problem of continuity can be seen from Figure 6.12 to have been removed by the inclusion of an overlapping boundary, as opposed to the simpler boundary model. The poor predictions of weld depth in the case of shallow welds are also improved through the use of the overlapping boundary. From the graphs in Figure 6.13 which compare all of the actual and predicted data points in each of the four areas of the welds, it is clear that training of the model for area D is not as successful as that of the other three models, in particular for the 270° measurement. This may be attributable to the different symmetries of the weld beads included in the database. However, a comparison of the spread of data points in Figures 6.4 and 6.13 demonstrates that the overlapping boundary model is the most successful approach.
Prediction of Multi-wire submerged arc weld bead shape using neural network modelling techniques
Prediction of Multi-wire submerged arc weld bead shape using neural network modelling techniques

Figure 6.12 - Comparison of the actual (solid line) and predicted (dashed line) images for the overlapping boundary neural network model, along with the actual measured data plotted against predicted data for each individual predicted image.
Prediction of Multi-wire submerged arc weld bead shape using neural network modelling techniques

Figure 6.13 - Comparison of actual data against predicted for all predictions, made by the four neural network simulations at (a) 0° (b) 90° (c) 180° and (d) 270° for the overlapping boundary model.

6.4.3 Overlapping Boundary Model - Input Relevance

An investigation of the relevance of each input in contributing to the variation in the output for the overlapping boundary model is presented in Figure 6.14. The four optimum models selected to predict the four separate regions within the overall bead shape were evaluated using the information stored in respect of the network weights and hyperparameters. Each of the four models shows a different dependence for the extent of the weld bead as a function of the various welding process parameters.
Figure 6.14a, for the central region containing the weld cap indicates that the current applied to the first and third wires, and the welding speed, are the most important input parameters. This is consistent with knowledge of the welding process; the third wire being responsible for the width of the cap in particular, and the current on the first wire affecting the overall degree of penetration. It has also been shown\textsuperscript{11} that an increase in welding speed, keeping all other parameters constant for multi-wire submerged arc welding, can be expected to reduce the penetration depth and produce a narrower weld bead, thus having a substantial effect on the width of the cap area of the weld.

**Figure 6.14** - Input relevance performed on the four neural network architectures of the overlapping boundary model, evaluating predictions at (a) 0° (b) 90° (c) 180° and (d) 270°
The contribution of the inputs to the shape of the base of the weld bead is described in Figure 6.14c. It can be seen that preparation depth has the largest influence on the output. The current, voltage and angle of wire 1 and, to a lesser extent, the spacing between wires 1 and 2, also show a strong influence on the output of this model. The voltage applied to the third wire is also predicted to be significant in this case.

For the two side areas of the weld, presented in Figures 6.14 (b) and (d) respectively, slightly different influences were determined on the shape of the weld bead. The current applied to wires 2 and 3, rather than the lead wire, were generally found to be the most important factors. This is consistent with the width of the weld bead being dependent on the extent of spread, determined in particular by the trailing wire. However, there was a variation in the influence of preparation angle, it being predicted to have a stronger influence in the $90^\circ$ position, but a much lower influence at the $270^\circ$ position. Electrode stickout was found to exhibit the opposite behaviour, i.e. a stronger influence at the $270^\circ$ position and a weaker one at the $90^\circ$ position. This difference may be attributable to the asymmetry of the welds contained in the database used for training purposes, and possibly to the method used for location of the origin of the weld bead described in section 2.2.

The examination of the relevance of the inputs to variation in the output, i.e. the extent of the weld bead shape, provides a useful insight. The overlapping boundary model appears to be following the expectations formed through prior knowledge of the welding process. Therefore, the level of confidence to which the use of multiple neural network models for different areas of the weld bead can predict the weld bead shape is high compared to a single neural network model for the weld bead shape as a whole.

6.5 Prediction Using Previously Unseen Data

A true test of the ability of a neural network is for it to be able to make predictions from previously unseen data to a high level of confidence. By selecting a sample weld image manufactured using parameters within the limits of the data used in training the neural network, and not previously presented to the network, it is possible to test the robustness of the model.
Figure 6.15 - Comparison of actual data against predictions made on previously unseen data for (a) the neural network model that considers weld bead shape as a whole and (b) the overlapping boundary neural network model.

Figure 6.15 illustrates the normalised data plotting actual against predicted data for (a) the initial model considering the weld bead shape as a whole and (b) the overlapping boundary model. The resulting weld bead shapes are given in Figure 6.16, which compares the actual weld bead shape with the two sets of predictions from the whole bead shape and overlapping boundary models overlaid. It can be seen that the overall shape of the weld bead is predicted well, including the bay region. The overlapping boundary model provides the best prediction of the asymmetry of the weld bead, and predicts the cap region very well, although there is a small difference in the depth of the weld bead.
6.6 Discussion

The complex relationships between weld process parameters and final weld bead geometry, together with the methods used in the prediction of weld bead shape, have been reviewed by McGlone\textsuperscript{1}. He discussed the use of a number of theoretical models, considering the problem from both a qualitative and quantitative perspective, and additionally noted that often the proposed methods require a high level of computation for their solution. Gunaraj and Murugan\textsuperscript{84, 85} have also considered a quantitative approach to important weld bead geometry parameters and the interaction of process control variables. They proposed analytical models to predict and optimise the welding process based on factorial techniques that can be utilised to investigate the effect of individual process parameters. The same authors also noted in a comparative study of the shape and area of heat affected zones for both bead-on-plate and bead-on-joint in submerged arc welding of pipes\textsuperscript{4} that the two were not directly comparable.

Lee et al\textsuperscript{100} investigated the occurrence of the 'bay' area in the SAW process, an important factor when considering the overall bead shape, and also the size of the heat affected zone as a function of welding parameters. Another approach to modelling weld bead shape is to use sophisticated heat flow analysis; Cho and Kim\textsuperscript{112} investigated this method for use with gas metal arc (GMA) welding of horizontal fillet joints. They considered an accurate approach to modelling the weld
thermal cycle, utilising 2D finite element models as a method of heat flow analysis in computing the base metal melting zones. Comparisons with experimental results showed that the proposed model was effective in predicting the weld bead shape, with the predicted melting zone of the base metal corresponding well with the experimental profile.

In addition to the approaches described above, there has also been previous work to utilise neural network techniques in the prediction of weld bead shape. Dilthey et al.\textsuperscript{103} used neural network techniques in the classification of weld bead geometry in GMA welding, mapping weld parameters to the resulting weld bead shape. Bead-on-plate weld geometry for GMA welding has also been considered by Chan et al.\textsuperscript{102}, who used procedure current, voltage and welder travel speed as inputs. Similarly Vitek\textsuperscript{91} used neural network modelling techniques in the prediction of the weld pool shape for pulsed laser welds, considering the bead area, bead depth, width and half width as his target variables. Chang et al.\textsuperscript{115, 125} compared the prediction of the shape of a spot weld using neural network techniques, earlier numerical models and finite element methods, concluding that a combined neural network and finite element method resulted in better predictions than stand alone techniques. Matsuyama\textsuperscript{82} used a trained neural network model in dynamic quality prediction of spot welds, comparing the voltage and welding current wave forms to predict the weld nugget size.

A key feature of previous work is that only a few parameters have been used to describe the weld bead; typically bead area, width and/or half width, depth, cap height, and then the weld bead shape is inferred from prediction of these parameters. In the current work, however, the entire weld bead shape has been predicted, giving an excellent representation of all the features of the weld bead, including asymmetry and the bay area.

The current research has also addressed issues concerned with shape of the weld bead in multiwire SAW welds. There has been little previous work in this area, with the majority of modelling approaches focussing on single wire welding. In a multiwire welding scenario, it is imperative that the wires all feed in to the weld pool such that the weld pool solidifies as a single mass. It is clear that there are a number of contributing factors to the final weld bead shape, including electrode geometry and weld process parameters. The dominant forces acting on the weld pool originate from the direction of movement of the welding head and a Lorentz force from the passage of the current through the liquid metal from each electrode. It is possible to visualise the lead wire as having a gouging action, and it has been shown in experimental
studies\textsuperscript{19,20} to be responsible for approximately 80-90\% of the penetration depth in the final weld bead shape. The gouging action is also clearly dependent on the wire angle. The current on the lead wire has been shown to be particularly important in affecting the penetration depth, and indeed the nature of the current (AC or DC) when compared with that on the other wires. The second wire increases the depth of penetration slightly and also acts to broaden the weld bead, whereas the third wire extends the penetration to 100\% whilst broadening the weld bead further, especially in the cap region of the weld.

The examination of the input relevance’s in the neural network models of bead shape are in excellent agreement with the experimental observations and have provided a useful insight, which concurs with metallurgical knowledge. Preparation depth was found to be an important factor in determination of the weld bead shape, as might be expected given that this controls the volume of weld metal to be deposited. The effect of welding speed was also of interest. It was found from the relevance of each input to variation in the output that if the speed increased, the width of the weld bead reduced, and vice versa, as expected\textsuperscript{11}. A number of the welding parameters, e.g. stickout, spacing, angle, were not found by the network to contribute to much of the variation in weld bead shape, probably due to the range of data used in the experimental database. However, the current on the lead wire was selected by the neural network as being particularly important in the overall depth of the weld bead, and the current on the third wire as important in the prediction of the horizontal extent of the weld bead, in agreement with experimental studies\textsuperscript{11,126}.

6.7 Refinements of the Weld bead Shape model

The work described in the previous section, although successful, used a relatively complex number of measurements to describe the weld bead shape. This complex method lends itself to applications in other modelling techniques, for example finite element methods; dependent upon a detailed description of the body to be modelled to ensure successful results. The large number of outputs that result from describing the weld bead shape in this way adds to the amount of error in modelling with a neural network.
6.7.1 Data used in modelling

It was decided following the rules of Occam's razor, chapter 4, to develop the weld bead shape model further to create a new model to predict a reduced number of essential weld bead shape descriptors. The main aim of simplifying and improving the weld bead shape prediction is to be able to apply the results to the prediction of weld metal mechanical properties; described in detail in chapter 7. It should also be noted that, in the manufacture of line-pipe, the quality control of the weld normally considers only a small number of measurements; cap height, bead width and penetration depth, as shown in Figure 6.17. By describing the weld bead width as two measurements from the origin to the points at 90° and 270° rather than a single measurement for the full width, any asymmetrical issues as far as weld bead shape are concerned will be accounted for. Additional measurements shown in Figure 6.18 were added to the inputs of the model described in Figure 6.17, to provide more detail about any flare region present. These additional measurements were incorporated to add more support to the key defining descriptive parameters, the extra measurements are; measurement and angle from the origin to the tangent on the bay area for both sides of the weld \((x_m, \phi_m)\). Measurements are taken on both sides of the weld, quantifying the flare region, in order to take into account any unbalance in the weld bead geometry.

![Figure 6.17 – Definition of measurements taken to describe the weld bead width, penetration depth and cap height](image)

Process control parameters are used to map against the outputs described above, enabling prediction of the weld bead shape using the reduced level of information available directly from the manufacturing environment compared to earlier work presented in this chapter.
A total of 164 data were available for the refined model of weld bead shape, due to the small quantity of data available once normalisation between -0.5 and 0.5, and randomisation were undertaken, data rows were only split into training and test data sets, omitting the validation set. For each modelling exercise inputs and outputs were kept constant, using the variation of the number of hidden units as an evaluative parameter.

In order to model the parameters described in Figures 6.17 and 6.18 a number of neural networks were trained considering the different areas of the weld; in order to reduce the number of output layer nodes. Large numbers of outputs contribute to higher error values when compared to the single output modelling, this is explained by increased complexity and the ‘average sum squared error’ (ASSE) evaluating the sum of the error on each output. The neural network modelling architectures were as described in Table 6.3 (a) showing the input parameters for each model and Table 6.3 (b) highlighting the output data being mapped. The possible combinations of input parameters mapped to output data can become overwhelming; from prior knowledge of the welding process four modelling architectures were chosen in order to evaluate whether it is possible to model the weld bead shape more accurately using the refined geometry descriptors, compared with the overlap and whole bead models.
Table 6.3 (a) – Definition of input parameters utilised in the refining of the weld bead shape modelling

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plate Thickness</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Preparation Angle</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Preparation Depth</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Current – Wire 1</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Voltage – Wire 1</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Angle – Wire 1</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Current – Wire 2</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Voltage – Wire 2</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Angle – Wire 2</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Current – Wire 3</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Voltage – Wire 3</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Angle – Wire 3</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Welder Travel Speed</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Vertical Stickout</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Spacing 1&gt;2</td>
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<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Wire Spacing 2&gt;3</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
</tbody>
</table>
### Table 6.3 (b) - Definition of output parameters mapped in the refining of the weld bead shape modelling

<table>
<thead>
<tr>
<th>Output Parameter</th>
<th>Model 1</th>
<th>Model 2</th>
<th>Model 3</th>
<th>Model 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cap Height</td>
<td>•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bead Penetration Depth</td>
<td>•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Width Measurement at 90°</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Width Measurement at 270°</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
</tr>
<tr>
<td>Measurement x₁</td>
<td></td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Measurement x₂</td>
<td></td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Angle φ₁</td>
<td></td>
<td>•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Angle φ₂</td>
<td></td>
<td>•</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

6.7.2 Results of modelling using the refined bead shape model

The error from the training and testing phases for models 1-4 are shown in Figure 6.19 (a) – (d) respectively, it is observed that a varied response is achieved depending on the bead geometry characteristic considered. In order to appreciate the training and test error values, on each individual model, for increasing model complexity each graph has been scaled relative to the modelling values; highlighting the shape of the error curve more clearly.

Through examination of the error values for all four models and further inspection of predictions made across training and test data domain, the optimum neural network architectures were obtained. The optimum number of hidden nodes for each model were; model 1 {9 hidden units}, model 2 {11 hidden units}, model 3 {5 hidden units}, model 4 {9 hidden units}. The optimum architectures of models 1-4 have been used to make predictions across both training and test data domains, shown in Figure 6.20 (a) – (e). The predictions made showed very poor correlation with the ‘y=x’ ideal, model 3 in particular showed relatively high values in training and testing and therefore badly predicted points are also seen from this model. Error bars have been removed from the graphs of prediction compared to measured data in Figure 6.20 (a) – (e) so as to clearly show the many predicted parameters. For the same purpose the predictions made using model 3 are displayed on two graphs, Figures 6.20 (c) and (d).
The output parameters modelled are not totally independent of one another; therefore by splitting
the shape into separate models vital information is missed. The best predictions are seen in
Figures 6.20 (a) and (e), both modelling the vertical penetration and in the case of model 1,
Figure 6.20 (a), the height of the weld cap. Comparison of predictions of the weld penetration
with those for the weld width and flare region show a significant difference in the level of
confidence that can be placed on the models. These results show that the penetration depth can
be classed as an independent characteristic, being independent of any other part of the weld bead
shape; defined by the characteristics of the lead wire and deposition of the first weld metal.
Perceived significance values, $\sigma_w$, showed little insight into why the modelling of the weld bead
graphs of the $\sigma_w$ values are not included.
shape in this way gives relatively poor results when compared to the overlap and whole bead
shape models used in previous sections, and therefore graphs of the $\sigma_w$ values are not included.
The lack of information from the $\sigma_w$ values, meant that it was difficult to evolve the models in
any structured manner, and it was decided that due to the lack of continuity between outputs that
the approach was not as good as that presented in earlier sections within this chapter.

Figure 6.20 – Predicted points compared with measured data for neural network models
considering various weld bead geometry characteristics, as described in Table 6.3; (a) Model 1,
(b) Model 2, (c) Model 3 weld width characteristics, (d) Model 3 flare region characteristics, (e)
Model 4
6.7.3 Discussion of the refinement of the weld bead shape model

An attempt to model weld bead shape parameters using a reduced number of geometry descriptors has been covered in this section. The principle behind the modelling approach stems from the fact that fewer measurements are taken in a manufacturing environment for quality control purposes and process monitoring. In later work these refined weld bead shape parameters are used in the prediction of weld metal toughness in order to keep the network architecture as simple as possible and the number of inputs to a minimum, while still sufficiently describing the weld bead geometry.

Comparing the results in section 6.7.2 with those for modelling with both overlap model and model considering the weld bead shape as a whole, it is clear that the neural networks for refined bead shape have has not been trained as well. The relationship between the input parameters utilised in modelling penetration, width, cap height and flare region hold a far simpler relationship to the weld geometry as a whole compared with individual measurements; meaningless on their own, though as part of the collective body have great importance. Vitek applied a similar technique to laser welds considering penetration, width, half width and area of the weld as output parameters. Similar problems were seen when training a network to predict the individual parameters, clearly observed in the results of the work.

Prediction of the angular measurement of the flare region is seen to be significantly poor, explained by the simple matter of data distribution, as there is little variation in the angular measurements taken to represent the weld flare. This leads to increased error in prediction of other outputs due to erroneous relationships being formed around the data. It is clear from the modelling of refined bead geometry descriptors that significantly better results can be achieved through modelling of the complete weld bead or overlapping regions. Comparison of the results in this section with all other results contained in this chapter gives strong evidence to this fact.
6.8 Conclusions

- It has been shown that neural network techniques can predict a weld bead shape to a high degree of confidence from manufacturing process parameters.

- The evidence suggests that the more measurements describing the weld bead shape profile, the better the accuracy of the predicted image. However, an efficient model can be made through the use of a smaller number of measurements for separate areas, with different neural networks being used to make predictions for such regions, providing that care is taken to ensure continuity at the overlapping points.

- Consideration of the relevance of each of the inputs to the output has also provided valuable insight into the effects of weld process parameters. The use of neural network models for the prediction of weld bead geometry has the potential for a detailed shape to be input into through-process models, rather than having to assume a shape from a limited number of defining parameters.

- Attempts have been made to utilise neural network techniques to predict key geometry descriptors around the weld bead; namely weld width, penetration depth, cap height and measurements with respect to the flare region of the weld. The work has shown that these measurements have very little relation to the welding process parameters on their own, with the predictions made showing a high level of uncertainty.

- The way in which weld bead shape is described with regards the modelling from welding process parameters has been found to be a key issue with respect to gaining good generalisation from the neural network models. The weld bead shape itself is a singular characteristic, though in order to define this in suitable terms for modelling it must be broken down into geometrical measurements defined throughout the chapter. It was found that penetration depth is classed as an independent shape characteristic, though all other geometrical parameters are dependent on the weld bead being classed as a whole or significant region of the weld. For example the weld width is determined by how much filler metal is deposited during the run of the lead wire and in some cases the second wire, thus is not independent and is related to the already determined penetration depth.
6.9 Chapter Summary

A significant problem faced by today's welding engineers, is the need to relate welding parameters to the quality of the finished weld. This is usually done by experience, and the need for many experimental trials, eventually leading to optimal welding parameters. Important characteristics in the evaluation of line-pipe seam weld quality are the weld bead shape and size, which can have a significant effect on the microstructure and mechanical properties of the weldment through heat flow effects.

This chapter describes the application of neural network techniques to the prediction of the outer diameter weld bead shape for 3-wire, single pass per side, submerged arc, line-pipe seam welds, using the weld process parameters as inputs. Novel methods of digitisation of weld macrostructures made under different experimental conditions, used in the training of the neural network, are discussed. The contribution of a particular welding process parameter (input relevance) to variation in the final weld bead shape is also considered. It is shown that it is possible to develop a neural network model that will predict the shape of an entire weld bead, without the need to assume it to be symmetric, with a relatively high degree of confidence.

Work on the refinement of the weld bead shape modelling using single or two output models to predict particular measurements, for example weld width, has revealed the dependent nature of weld bead shape descriptors. The penetration depth, produced through gouging effects of the lead welding wire, was found to be predicted well revealing the independent nature of this shape measurement. All other measurements are defined not only by the welder set-up but by any previous weld metal laid down in that run, and thus all measurements are dependent of one another and weld bead geometry must be classed as a whole. This has shown that the published work utilised the best method for successfully predicting the weld bead geometry. This is further backed-up by the excellent results achieved.
Chapter 7 – Modelling of weld metal mechanical properties using neural
network techniques

7.1 Introduction

The design of any commercially produced weld is usually carried out using skills and knowledge accumulated through experience gained from costly, time consuming experimental trials. Any attempt to simplify this methodology through quantitative modelling must recognise the complex nature of the weld metal and processes involved. Blind procedures such as regression analysis and neural networks can reveal new regularities in the data by closely mimicking human experience through learning or being able to recognise correct science. Ideally modelling should be based on firm physical principles that, once established, can be used with greater confidence and are capable of predicting new phenomena.

Models based on metallurgical assumptions are less numerous in the case of weld metal than those using so-called blind techniques. With any modelling of the weld metal mechanical properties it is important to determine the contributory factors from the various areas of the welding process; namely chemistry, microstructure and thermal cycle outlined in Figure 7.1. It can be seen that the relationships between the various parameters contributing to the weld metal mechanical properties are highly complex, and therefore make the modelling of weld metal mechanical properties a difficult task using physical principles. Therefore, a preferred method would be to train a neural network using many examples, developing a suitable model in much the same way a welding engineer would develop his knowledge over time.

Throughout the literature many attempts have been made to model weld metal mechanical properties using neural network techniques. Bhadeshia et al\textsuperscript{64} developed a Bayesian neural network analysis technique for the prediction of C-Mn steel arc weld toughness. The neural network used considered chemical analysis, microstructural constituents, welding process identification and, most importantly, the yield strength (YS). The use of YS for the approach in this chapter would inappropriate because it is desired that mechanical properties be predicted from information available from a production perspective i.e. before a weld is manufactured. Similar modelling to that of Bahdeshia was carried out by Lalam et al\textsuperscript{99}, this time predicting the
temperature-toughness characteristics of the steel welds. Interestingly the yield strength was utilised as an input parameter in this work also.

![Flow chart showing how the mechanical properties of weld metal are determined, adapted from Bourges et al.](image)

Cool et al.\textsuperscript{129} used neural network techniques in the prediction of steel weld metal yield strength and ultimate tensile strength (UTS). The models for YS utilised weld metal chemistry and heat input, including also inter-pass temperature and tempering temperatures. Modelling of UTS maintained a similar approach, although values of YS were included as inputs. Inclusion of YS as an input when modelling UTS seems flawed as both values are measured during the same procedure. Tensile strength was also modelled in the work of Lalam et al.\textsuperscript{97, 98} using weld metal chemistry, heat input and any information about post weld heat treatment (PWHT).

When modelling any quantifiable parameter using neural network techniques, the accuracy is determined to a great extent by the volume and quality of data presented to the network. The data made available for the work in this thesis had sufficient quantity and quality for previous modelling exercises, however upon modelling of mechanical properties the amount of quality data was found to be lacking. This is attributed to the relationship between an increase in number of variables and the decrease in volume of quality data available. During the modelling of weld metal toughness it was found that to get around the fact that there was a small quantity of data available, the temperature at which toughness has been tested could be used as an input.
parameter, thus increasing the amount of data available by allowing repetition of other parameters alongside the temperature flag.

Although the amount of data was lacking with regards other weld metal mechanical property characteristics, an attempt was made to model the weld metal hardness and tensile strength. Key parameters, for example the weld metal microstructure, were omitted from the modelling algorithm for both hardness and UTS, as certain key parameters limited the maximum data available to the work. The major work in this chapter applies to the modelling of weld metal toughness using a variety of input variables including weld metal chemistry, weld process parameters and weld bead geometry, with more limited consideration of other mechanical properties. The techniques used in the chapter consider only information available from a manufacturing standpoint.

7.2 Definition of Weld Charpy Toughness

The toughness of a material is defined as the energy absorbed in fracture. There are several ways to measure toughness, the most common is by impact testing in which the material is struck with a hammer and the energy absorbed by the material in fracture is measured. Impact toughness testing is mainly a ranking technique; a brittle material is defined as absorbing little energy whereas a tough material will absorb large amounts of energy during the fracture process. Metals generally have a high toughness, whereas glasses and ceramics have low toughness values. Taking impact tests at differing temperatures enables the material behaviour to be mapped. The welds in the database were impact tested at differing temperatures from $-130^\circ\text{C}$ to $60^\circ\text{C}$, and by incorporating this value into the modelling algorithm, input parameters such as plate thickness and wire stickout were repeated for each Charpy test. The repetition of parameters allowed the number of data to increase to over 1000 for use with the neural network, whereas only around 150 data would be available without the use of different test temperatures.

The Charpy toughness data considered in this modelling are weld metal toughness values taken from the outer diameter weld (OD) of one pass per side multiple wire submerged arc welds from steel line pipe. Outer diameter welds are considered here due to the ease in which information regarding shape and area of the weld bead can be obtained, unlike with inner diameter (ID) welds which are partially consumed by overlaying the outer diameter welding. Outer diameter weld metal toughness tests are also known as a 2 mm sub-surface Charpy tests; samples received
from the mill are measured and positioned before being machined exactly 2 mm from the OD. The sample is then turned and machined from the ID leaving a test specimen 10 mm wide, and etching is used to locate the position of the weld metal in the sample. The notch for a weld metal test samples 100% weld metal down the centre line of the weld as described in Figure 7.2.

Figure 7.2 – Definition of the machining position for Charpy toughness test samples for outer diameter line-pipe welds

The Charpy toughness of the weld metal relies on many parameters from the welding process; these parameters are closely controlled to obtain a ‘good’ weld metal microstructure containing a high ratio of acicular ferrite relative to other microstructural constituents. A good model for the weld metal toughness therefore must consider chemical composition, heat input and cooling rate of the weld metal:

- Chemical composition: Governed by the composition of plate, wire electrodes and flux additions.
- Heat Input: Governed by the amps and volts across all welding electrodes and the welder speed.
- Weld Cooling Rate: Governed by ambient temperature or forced cooling, heat sink (amount of parent material/plate thickness absorbing heat) and weld bead shape.
7.3 Initial work on the modelling of weld metal mechanical properties using neural network techniques

Initial work carried out using a combination of chemical composition and weld metal microstructure to predict weld metal toughness, yielded good results. OD weld metal only is considered throughout this chapter to enable comparison of results using varied input architectures. The inputs used for the initial model were:

- Weld wt.%
  - C
  - Mn
  - Si
  - Al
  - P
  - S
  - N
  - O
- Acicular Ferrite (AF%)
- Primary Ferrite (PF%)
- Charpy Test Temperature

Data were normalised between the limits -0.5 and 0.5, randomised then split as outlined in Table 7.1. The pre-processed data were then used to train a set of neural network models keeping inputs the same, using the variation in the number of nodes in the hidden layer as the evaluating factor. To ensure the neural network gained sufficient convergence 1000 Markov chain Monte Carlo steps were used.

<table>
<thead>
<tr>
<th>Data Type</th>
<th>Number of Data Sets</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training</td>
<td>500</td>
</tr>
<tr>
<td>Test</td>
<td>500</td>
</tr>
<tr>
<td>Validation</td>
<td>99</td>
</tr>
<tr>
<td>Total</td>
<td>1099</td>
</tr>
</tbody>
</table>

Table 7.1 – Outline of data separation for use with modelling weld metal toughness from weld metal chemical composition and weld microstructure.
7.3.1 Results of first attempts at modelling weld metal toughness

The errors on training and testing for the modelling of Charpy toughness as defined in section 7.3 are shown in Figure 7.3. From these error values the optimum neural network architecture was determined to contain 7 hidden units. Figure 7.4 represents the predicted weld toughness compared with the actual weld toughness data using a neural network model containing 7 hidden units across the training data domain, Figure 7.4 (a), test data domain, Figure 7.4 (b), and the validation data domain Figure 7.4 (c). The predictions made using training and test data enabled the determination of how well the training and testing phases had been undertaken. The use of a validation data set evaluates how well the neural network can make predictions using previously unseen data taken from the same data distribution as the training and test data sets. The graphs in Figure 7.4 show a good correlation with the ideal \( y = x \) relationship between actual and predicted data, seen across all data domains.

![Image of Figure 7.3 showing error on training and testing data for a neural network model mapping weld metal chemistry and weld metal microstructural constituents against weld metal toughness.](image-url)

**Figure 7.3** – Error on training and testing data for a neural network model mapping weld metal chemistry and weld metal microstructural constituents against weld metal toughness.
Modelling of weld metal mechanical properties using neural network techniques

Figure 7.4 - Predicted toughness against actual toughness for a neural network model mapping weld metal chemistry and weld metal microstructural constituents against weld metal toughness, containing 7 hidden units for (a) training set, (b) test set and (c) validation set.

7.3.2 Evaluation of neural network modelling of weld Charpy toughness from weld metal chemistry and weld metal microstructure constituents

In Figure 7.5 (a) and (b) the weights on connections between the input and output layer, and the average of the weights between the input and hidden layer are shown respectively, for a 7 hidden unit neural network architecture. The information displayed in Figure 7.5 (a) and (b), gives supporting evidence as to the level of confidence at which the neural network model can predict weld metal toughness from the input parameters being evaluated. Considering the input to output layer weightings, it is seen that the test temperature stands out as having the greatest influence, which is to be expected as test temperature is the defining flag parameter for repeating all other input data.
Figure 7.5 (a) – Weights on connections between input and output layer for a 7 hidden unit neural network architecture, modelling weld metal Charpy toughness from weld metal chemistry and microstructure.

Figure 7.5 (b) – Average weights on connections between input and hidden layer for each individual input parameter, for a 7 hidden unit neural network architecture, modelling weld metal Charpy toughness from weld metal chemistry and microstructure.
An investigation of weightings placed on the connections between the input and hidden layer, identifies the influence of the input parameters that are related to the output through more complex relationships than those identified through the connections from input to output layer. The information available through examination of input to hidden layer weights becomes quite substantial therefore by taking an average across all the connections for a particular input parameter, the influence on the model output can be determined. Weightings across the connections between input to hidden layer for each individual input parameter for a neural network model of the weld metal toughness shown in Figure 7.5 (b), highlights the acicular ferrite input to carry most influence with a relatively smaller influence spread over some chemical elements. To obtain optimum weld metal toughness it is essential to maximise the amount of acicular ferrite, therefore it is expected that the level of acicular ferrite in the model be strongly related to the output toughness. Other input parameters showing relatively high weightings are; weld wt.% O, weld wt.% N, weld wt.% Al, weld wt.% S and test temperature. Test temperature is expected to show some level of influence as described in the input to output weights, with other weld metal chemical content parameters also expected to show some weighting as they are related to the formation of the inclusions found within the weld metal. Inclusions act as nucleation sites for the formation of the acicular ferrite matrix.

7.4 Evolution of the neural network model for weld metal toughness

The approach described in section 7.3 proved to be successful although the parameters used in modelling were not readily comparable to the known information obtainable during the weld manufacture process. The information available at the manufacturing level can be quite overwhelming and in some cases related to the mechanical properties through highly complex relationships involving parameters not available or recorded during the manufacturing process. Methods were required to reduce this data; as with the model in section 7.3 where weld metal chemistry is utilised rather than the use of plate, wire and flux chemistry to describe the same inputs.
Two methods of attack were proposed following a microstructural route or a weld process and bead shape method, using committees of models to progress from manufacturing inputs to the desired output:

1) Prediction of microstructural constituents and weld metal chemistry from welding process parameters, input materials and consumables, using outputs of several models to produce the above input parameters.

2) Predictions of weld metal toughness using outputs from neural network models for weld metal chemistry and weld bead shape (thus considering cooling rate factors, linked to the formation of the weld metal microstructure), alongside process parameters. This has the potential to produce a model predicting everything solely from welding process parameters.

The success of the two modelling approaches mentioned above is determined to a great extent by the quality of data output by the 1st level of neural network models. The modelling in approach 1 would consider the use of models developed in chapter 5, maintaining the same approach as described in section 7.3 utilising predicted rather than measured values.

7.4.1 Addition of simple welding process parameters to the chemistry model

To evaluate the effects of certain parameters a solely chemistry input model was developed removing the information regarding microstructural constituents, thus evaluating the modelling capabilities of the neural network when obvious parameters are removed. Once again the same quantity of data as defined in section 7.3 was available to the modelling, normalising between the limits -0.5 and 0.5, and randomising before the data was split as outlined in Table 1. The pre-processed data were then used to train a set of neural network models keeping inputs the same and using variation in the number of nodes in the hidden layer as the evaluating factor. To ensure the neural network gained sufficient convergence 1000 Markov chain Monte Carlo steps were used.
Modelling of weld metal mechanical properties using neural network techniques

In Figure 7.6 the results of error determination across the training and test phases are displayed; the optimum architecture is seen to contain 11 hidden units. Predictions on validation data made with the neural network model containing 11 hidden units are shown in Figure 7.7, showing a good correlation with the actual toughness data being mapped.

Investigation of the weights across the neural network for the connections between input to output layer and input to hidden layer are shown in Figure 7.8 (a) and (b) respectively. Across the input to output weightings the test temperature and amount of sulphur present in the weld metal appear to have the largest influence. Test temperature is expected, as this is the flag input for all other repeated inputs within the data. Sulphur is classed as an impurity, along with nitrogen and phosphorous, contributing to lowering fracture toughness in steels. Once again impurities show a high influence when looking across the weighting in the input to hidden layer, with the carbon content of the steel also showing strong influence as expected.

Figure 7.6 – Error on training and testing data for a neural network model mapping weld metal chemistry against weld metal toughness.
Modelling of weld metal mechanical properties using neural network techniques

Figure 7.7 - Predicted toughness against actual toughness for a neural network model mapping weld metal chemistry against weld metal toughness, containing 11 hidden units. Considering previously unseen data.

Figure 7.8(a) - Weights on the connections between the input layer and the output layer for a neural network architecture containing 11 hidden units, for the modelling of weld metal toughness considering only weld metal chemistry and test temperature as inputs.
Figure 7.8(b) – Average weights on the connections between the input layer and hidden layer for a neural network architecture containing 11 hidden units, for the modelling of weld metal toughness considering only weld metal chemistry and test temperature as inputs

### 7.4.2 Addition of Process Parameters

The next stage in the evolutionary process was to add inputs to those discussed above representing the heat input from the welding process, defined below:

- **Plate thickness** – the size of plate is directly related to the heat absorption, and the rate at which heat is removed from the weld area.
- **Welder speed** – faster welding speeds, means a lower heat transfer to the weld metal
- **Heat Input** – calculated from the volts and amps applied across each welding wire

Choosing the measured heat input, calculated from the electrical input to the individual welding wires keeps the number of inputs to a minimum, simplifying matters, and therefore giving the model more chance of converging on correct results. Results of training and testing errors for varying the number of hidden units in the neural network architecture can be seen in Figure 7.9, the error on these training and test sets are just as low as those seen in section 7.4.1. Predictions made using a 10 hidden units architecture on previously unseen data can be seen in Figure 7.10. Although a good correlation between actual and predicted points can be seen some outliers are
also present. Furthermore, a comparison of results in Figure 7.10 with the work in section 7.3, shows no significant gain, although this could be due to the rather simple descriptors used for the welding process.

Figure 7.9 – Error on training and testing data for a neural network model mapping weld metal chemistry, plate thickness, welder speed and heat input against weld metal toughness.

Figure 7.10 – Predicted toughness points, made using validation data, compared with actual toughness values for a neural network model mapping weld metal chemistry, plate thickness, welder speed and heat input against weld metal toughness, containing 10 hidden units.
Figure 7.11 (a) and (b) show the weightings placed on connections between input and output and the average weightings for each individual input parameter placed on the connections between input layer and hidden layer respectively. Investigation of the results displayed in Figure 7.11 (a) and (b) show that the addition of these new input parameters do give a significant influence on the neural network modelling. This is expected as the three added parameters reflect issues as regards the thermal cycle being undertaken and are related to the formation of the weld metal microstructure. As with modelling using solely chemical inputs, in section 7.4.1, there is a similar relative weighting on the same chemical inputs for both weightings across input to output connections and input to hidden layer connections. No shift in weighting is seen as expected with the weld metal chemistry inputs, as identifiable chemical elements showing a high relative influence play a vital role as far as reduction of oxides and formation of inclusions.

Figure 7.11(a) – Weights on connections between input layer and output layer, for a neural network with architecture containing 10 hidden units, modelling weld metal toughness from weld metal chemistry and simple welding parameters
Figure 7.11(b) – Average weights on connections between input layer and hidden layer for each individual input parameter, for a neural network with architecture containing 10 hidden units, modelling weld metal toughness from weld metal chemistry and simple welding parameters

7.4.3 Welding Process Parameters Model

In order to investigate the use of a more complex combination of welding parameters, evolving from the use of just heat input, plate thickness and welder travel speed, weld metal chemistry was omitted so as to determine the important weld process parameters in prediction of toughness. A total of 940 data were available for input to the basic comparative neural network model, using test temperature to repeat manufacture data from 178 submerged arc welds. As with all modelling this data was normalised between the limits \([-0.5, 0.5]\), randomised then divided to form training, testing and validation sets. To ensure the neural network gained sufficient convergence 1000 Markov chain Monte Carlo steps were used. The inputs considered in the mapping of the weld metal toughness to weld process parameters were:

- Plate Thickness
- Weld Preparation Angle
- Weld Preparation Depth
- Amps – Wire1, Wire2, Wire3
- Volts – Wire1, Wire2, Wire3
- Wire Angle – Wire1, Wire2, Wire3
- Welder Speed
- Wire Vertical Stickout
- Wire spacing - Wire 1 and Wire2
- Wire Spacing - Wire 2 and Wire3
- Toughness Test Temperature
Figure 7.12 shows the average sum squared error compared with increasing number of hidden layer nodes for the model for weld metal toughness, the results show that training error decreases with increased complexity, although there is a finite limit to this gain on the test error with the best model containing 9 hidden units. Predictions made by the best neural network model using validation data are shown in Figure 7.13. It is seen in Figure 7.13 that the model shows a good ability to predict the trend of toughness from the process parameters, although a high level of uncertainty is present, identifiable due to the large number of badly predicted points.

**Figure 7.12** – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of Charpy toughness without the use of weld bead shape parameters.
Figure 7.13 – Prediction of Charpy toughness at varied test temperature using weld process parameters using validation data, with a neural network architecture containing 9 hidden units.

Figure 7.14 (a) – Weights on connections between input and output layer, for a neural network architecture containing 9 hidden units, modelling weld metal toughness using just weld process parameters as inputs.
Figure 7.14 (b) – Average weights on connections between input and hidden layer for each individual input parameter, for a neural network architecture containing 9 hidden units, modelling weld metal toughness using just weld process parameters as inputs

An assessment of the weights on input to output connections and input to hidden layer connections, shown in Figure 7.14(a) and (b) respectively, doesn’t throw much light on the input parameters having the most influence on the model output. The uncertainty as to the most influential parameters is reflected in the predictions made on validation data, shown in Figure 7.13. Test temperature can be seen to have a high level of influence across the input to output layer connections, however, it is not the only responsible parameter. The only other modelling parameters that have any significant influence on the modelling outcome are the currents applied to wires 2 and 3 respectively. This can be explained by the heating effect of the current applied to the two trailing wires, which elevate the weld pool liquid metal to the maximum temperature before solidification and final formation of the eventual weld metal microstructure. Weld metal chemistry is expected to play an important role in the modelling of weld metal toughness, and therefore if used as an input parameter then it would be expected to reduce the weighting values from the current on wires 2 and 3.

The values of modelling errors, predictions on validation data and input relevance testing reveal very little as regards the algorithm for weld metal toughness when related to just the welding process parameters. This is therefore indicative of the need for weld metal chemistry in the input
layer when modelling the toughness of the weld. More importantly, the microstructure must be considered, especially the acicular ferrite content, together with other elemental additions and the applied heating cycle.

7.5 Introduction of weld bead shape into the modelling of toughness

The next phase in the evolution of the model for weld metal toughness was to consider the use of weld bead shape as an input, which is directly related to the cooling rate of the weld\textsuperscript{130}. Weld bead shape is clearly not readily available from welding process information and therefore the ultimate aim is to produce a neural network model which can utilise input data regarding the weld bead shape from the output of another neural network model. It was decided to use actual measured data in the development phase to evaluate the best neural network modelling architecture because the output of neural network models for prediction of weld bead shape are not 100\% robust in their predictions.

The toughness of weld metal is strongly influenced by its chemical composition and microstructure; determined by the consumables used, the presence of inclusions, and the welding parameters especially process temperature and cooling rate. The cooling rate is directly related to the area of the weld bead shape being manufactured, and the thickness of the parent plate in question. Earlier work in this chapter has considered modelling weld metal toughness using weld metal chemistry as input parameters, and showed a good correlation between predictions and actual data. In the following section the use of simple weld bead shape parameters will be added to chemical analysis values and any differences noted, in terms of prediction of toughness.

7.5.1 Initial bead shape model

The total area of the weld bead, approximated using the triangles formed by the polar measurements, was added to the modelling architecture described in section 7.4.2, creating a 13 input model. The data were normalised between the limits \(-0.5\) and \(0.5\), then randomised before separation into training, test and validation data sets. In total 665 data were available for the modelling exercise, 300 data were used in training and 300 for testing with 65 being kept aside for validation of the neural network. All inputs and outputs were kept constant, varying the number of hidden units as an evaluative process, using 1000 Markov chain Monte Carlo steps in an effort to gain good convergence in training and testing. The reduction in the quantity of data
available, when compared to earlier section in this chapter, is a good example of data quantity reducing with the increased number and complexity of data inputs.

The average sum squared error from the training and testing phases is shown with increasing complexity of the neural network architecture in Figure 7.15. It is seen that beyond 13 hidden units the training error increases rapidly caused by a need for more steps in the Markov chain Monte Carlo process. Increases in the number of Markov chain Monte Carlo steps would be inefficient as far as computing time is concerned because the test error is already small and does not show any significant improvement beyond 13 hidden units. The optimum neural network architecture was found to contain 11 hidden units, determined using values of training and test error. Predictions made using the optimum 11 hidden units neural network architecture on validation data are found in Figure 7.16; these predictions show a good correlation with the ‘y=x’ ideal relationship between actual and predicted points. Compared with modelling in section 7.3 the results are seen to show a slightly lower level of confidence, explained by the use of the new input parameter defining the bead shape loosely, while increasing the complexity of the blind model.

Figure 7.15 – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of Charpy toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area as inputs
Figure 7.16 – Prediction of Charpy toughness at varied test temperatures using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area as inputs from validation data for a 11 hidden units neural network architecture.

An investigation of the weightings placed on the connections between input and output layer and the average weights for each input parameter between input and hidden layer are displayed in Figure 7.17 (a) and (b) respectively. As expected, throughout the modelling of weld metal toughness, the largest weighting is placed on test temperature for connections between input and output layers. Smaller relative weightings are placed on weld wt.% O, weld wt.% Mn and welder travel speed in that order, with all other weightings carrying relatively insignificant values.
Figure 7.17 (a) – Weights on connections between input and output layer, for a neural network architecture containing 11 hidden units, modelling weld metal toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area as inputs.

Figure 7.17 (b) – Average weights on connections between input and hidden layer for each individual input parameter, for a neural network architecture containing 11 hidden units, modelling weld metal toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area as inputs.
More complex issues evaluated through the connections between input layer and hidden layer show that the most significant weightings are placed on weld wt.% Al, plate thickness and weld wt.% Si, in that ranking order. Thickness would be expected to be important because it is proportional to the size of heat sink available. Aluminium and silicon are considered to be deoxidising additions.

7.5.2 Evolution through increase in weld bead shape descriptors

Given the limited success in adding a simple representation of weld bead area it was decided to add more descriptors with regards the weld bead shape to provide more information between the inputs and outputs with respect to the heat distribution at the weld. A total of 17 inputs were therefore contained in the input layer:

- Plate thickness
- Welder travel speed
- Measured heat input
- Weld wt.% C
- Weld wt.% Mn
- Weld wt.% Si
- Weld wt.% Al
- Weld wt.% P
- Weld wt.% S
- Weld wt.% N
- Weld wt.% O
- Test Temperature
- Weld bead Area
- Cap Height*
- Bead Penetration*
- Measurement from origin at 90°*
- Measurement from origin at 270°*

*As defined in Figure 7.18

![Diagram of weld bead shape](244)
The data quantity remained the same as described in section 7.5.1 following the same thorough pre-processing regime. The errors on training and testing displayed in Figure 7.19 reveal the optimum neural network architecture to contain 10 hidden units. Predictions made using the optimum neural network, containing 10 hidden units shown in Figure 7.20. It can be seen that the output results show an improvement on the model in section 7.6.1, which used only area to describe the weld bead shape. Predictions show that by using more information to describe the weld bead shape, a more robust relationship can be mapped between the inputs and the weld metal toughness. However, it is seen in the graph in Figure 7.20, that for points which do not fit well to the ‘y=x’ ideal line, large error bars are present indicating that some overfitting is occurring. The overfitting is easily explained by the high number of inputs to outputs being modelled by the neural network, and suggests that the model is over complicating the relationships in the data presented to it.

![Graph showing error vs. hidden units](image)

**Figure 7.19** – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of Cv toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area with dimensions as inputs.
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Figure 7.20 – Prediction of Charpy toughness at varied test temperature using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area with dimensions as inputs from validation data for a 10 hidden units neural network architecture

Figure 7.21 (a) – Weights on connections between input and output layer, for a neural network architecture containing 10 hidden units, modelling weld metal toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area with dimensions as inputs
Figure 7.21 (b) – Average weights on connections between input and hidden layer for each individual input parameter, for a neural network architecture containing 10 hidden units, modelling weld metal toughness using a combined heat input with a reduced number of weld process parameters, weld metal chemistry and weld bead area with dimensions as inputs.

The test temperature was again found to carry the heaviest weighting on connections between input and output layer, for all previous modelling in this chapter, though input weightings displayed in Figure 7.21 (a) show this to have very little weighting in relative comparison to the other input parameters. The use of 17 inputs is complex relative to other modelling architectures and is attributable for the shift in weighting from test temperature. Information about weighting values placed on connections between input and output layer highlight the wt.% C and plate thickness as the two heavily weighted parameters, all other parameters carrying relatively insignificant weightings. The wt.% C is directly related to the toughness of steel, the increase in C content of the weld metal is almost a linear relation to the decrease in impact energy of steel. It is not expected that wt.% C and plate thickness should overtake the test temperature as far as weightings are concerned, especially as test temperature is paramount to the data structure being presented to the neural network.

Test temperature is shown to carry the highest influence across the weightings for each individual input parameter on connections between input and hidden layers. Influence of the area and dimensions of the weld bead shape are classed as relatively low, along with welding process...
input parameters the opposite of what was expected. Of the chemical elements being used in modelling the data, weld wt.% N, wt.% Si, wt.% Mn and wt.% S show the largest influence in that ranking order, weld wt.% N having by far the highest of the rankings.

7.5.3 Validating the use of the re-defined weld bead shape model using measured values

Considering the weld bead shape descriptors defined in the previous section new parameters were added from the weld bead shape model described in chapter 6 section 6.7. Two input architectures were considered the first using the eight weld bead shape descriptors plus a single value for weld bead area and secondly with the area omitted. Measured values were initially used to prove the validity of the modelling method, using the parameters described below. Following filtering and cleaning of the data a total of 665 data were available, normalisation of the data was undertaken, scaling between the limits \(-0.5\) and \(0.5\) followed by randomisation and splitting into training, test and validation data sets.

**Inputs**

- PlateThickness
- Welder Travel Speed
- Measured Heat Input
- Weld wt.% C
- Weld wt.% Mn
- Weld wt.% Si
- Weld wt.% Al
- Weld wt.% P
- Weld wt.% S
- Weld wt.% N
- Weld wt.% O
- Test Temperature
- Cap Height (at 0°)
- Bead Penetration (at 180°)
- Measurement at 90°
- Measurement at 270°
- Measurement \(x_1\)
- Measurement \(x_2\)
- Angle \(\phi_1\)
- Angle \(\phi_2\)

NB: - The total area of the weld bead shape was added to the list above as an input in one modelling exercise and removed from the other, used as a comparison of the need for this input.

The error on training and testing data are compared in Figure 7.22 and show that the inclusion of weld bead area causes the level of error in training to increase probably as a result of the increase
in the number of inputs when area is added into the algorithm. The optimum weld architecture for both models contained 13 nodes in the hidden layer, and a comparison of the predictions made by each model using validation data are shown in Figure 7.23 (a) model using weld bead area and (b) model with weld bead area omitted. It must be noted that due to data being randomised the validation data used with each model are completely different.

![Figure 7.22](image)

Figure 7.22 – Average sum squared error shown with increasing complexity of the neural network architecture for the modelling of Charpy toughness using parameters from a re-defined weld bead shape model with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs, comparing (a) a model using weld bead area as an input, and (b) a model omitting weld bead area from the input parameters

The graphs in Figure 7.23 (a) and (b) clearly show that the inclusion of the weld bead area has a negative effect on the accuracy with which predictions can be made using a neural network model considering the inputs defined in this section mapped to weld metal toughness. The predicted points in Figure 7.23 (b) fit the ‘y=x’ ideal relationship between actual data and predicted data much closer than in (a) with far less outliers. An investigation of the weightings placed on the inputs shown in Figure 7.24 and 7.25, highlight where the differences occur from the introduction of weld bead area into the modelling equation.
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Figure 7.23 (a) – Comparison of actual data against predicted data, for a neural network model for weld metal toughness containing 13 hidden units, using parameters from a re-defined weld bead shape model including weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs

Figure 7.23 (b) – Comparison of actual data against predicted data, for a neural network model for weld metal toughness containing 13 hidden units, using parameters from a re-defined weld bead shape model omitting weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs
Modelling of weld metal mechanical properties using neural network techniques

Figure 7.24 (a) – Weights on connections between input and output layer, for a neural network architecture containing 13 hidden units, modelling weld metal toughness using parameters from a re-defined weld bead shape model including weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs.

Figure 7.24(b) – Average weights on connections between input and hidden layer for each individual input parameter, for a neural network architecture containing 13 hidden units, modelling weld metal toughness using parameters from a re-defined weld bead shape model including weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs.
Figure 7.25 (a) – Weights on connections between input and output layer, for a neural network architecture containing 13 hidden units, modelling weld metal toughness using parameters from a re-defined weld bead shape model omitting weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs.

Figure 7.25 (b) – Average weights on connections between input and hidden layer for each individual input parameter, for a neural network architecture containing 13 hidden units, modelling weld metal toughness using parameters from a re-defined weld bead shape model omitting weld bead area with a combined heat input, reduced number of weld process parameter and weld metal chemistry as inputs.
A comparison of weightings placed on the connections between input and output layer for the model including weld bead area, shown in Figure 7.24 (a), and the model omitting the weld bead area from the input data, shown in Figure 7.25 (a) highlight the reasons for differences in predicting weld metal toughness. Both models, as expected, place the highest weightings on the test temperature, although where weld bead area is included this weighting is considerably lower. Weld bead area is seen to carry a relatively high weighting in comparison to other input parameters in Figure 7.24 (a), removing weighting from other more important parameters, for example the bead penetration ($x@180$) is shown to have a relatively high weighting in the model omitting weld bead area, this is much reduced in the model containing weld bead area. The weld bead area is directly linked to the other weld bead measurements and is theoretically not required.

Weld bead area is found not have as much of an effect on the modelling outcome when the weightings placed on the connections from each input parameter between input an hidden layer are considered. The average weightings of the connections from each input parameter to the hidden layer nodes are shown in Figure 7.24 (b) for the modelling including the weld bead area, and in Figure 7.25 (b) for modelling without the weld bead area as an input parameter. Both models show a good correlation in that they place the largest weighting on the weld metal nitrogen content. Other parameters are weighted differently, with the model omitting weld bead area as an input shows a better weighting pattern, with far more key parameters being seen to be weighted, than that of the model including weld bead area. The weightings shown in Figure 7.25 (b) for the model omitting weld bead area shows a good spread of weighting over chemical elements important to the toughness rating that will be achieved in the particular weld in question. The elements having high weightings are carbon (C), sulphur (S), aluminium (Al) and oxygen (O). Weighting over the test temperature is also observed to be relatively high as is expected being paramount to the data formation used in these modelling exercises. It is interesting to note that the model places a significant weighting on the measurement $x_1$, identifying the flare region, but not on its twinned measurement $x_2$. This signifies a pattern having been found in this data, though not one that can be related to metallurgical phenomena, and therefore points to the fact that the level of confidence with which the model including weld bead area predicts weld metal toughness is low.
7.6 Modelling of weld metal toughness using a committee of neural network models

In order to demonstrate that a committee of neural networks could be utilised to predict weld metal toughness using only information available from a manufacturing perspective, a strategy was then developed using input data gained from predictions made using the chemistry and acicular ferrite models described in chapter 5. Data were filtered so as to ensure that the same welds were being considered when predicting the weld metal chemistry and weld metal acicular ferrite content; a total of 99 welds were available following this process. In order to obtain a correlation with the previous trained neural network models to be used for prediction, the data were normalised using the values obtained for the data used in training the respective models. The prediction of weld metal chemistry was carried out using the multiple output model defined in chapter 5 section 5.4.3 using an 8 hidden unit neural network architecture. The prediction of the acicular ferrite content of the weld was undertaken using the model described in chapter 5 section 5.6.1, utilising a hidden layer containing 10 nodes. The predictions made from both these models would then be fed into the input layer of a neural network model for Charpy toughness described in Figure 7.26. Plots of the predicted points, against the actual data comparisons, for the data to be utilised in a model for weld metal toughness are shown in Figure 7.27.
Modelling of weld metal mechanical properties using neural network techniques

Multiple Output Chemistry Model

![Diagram of Multiple Output Chemistry Model]

Acicular Ferrite Model

![Diagram of Acicular Ferrite Model]

*Figure 7.26* – Schematic showing the flow of data to the neural network model for weld metal toughness, using predicted values of weld metal chemistry and acicular ferrite as inputs.
Figure 7.27 –
Predicted data for use in the neural network model for weld metal toughness.
Predicted weld metal:
(a) wt.% C
(b) wt.% Mn
(c) wt.% Si
(d) wt.% Al
(e) wt.% P
(f) wt.% S
(g) wt.% N
(h) wt.% O
(i) % AF
The predicted data in Figure 7.27 shows a varying level of accuracy for the different predicted parameters, as was seen in the work in chapter 5. Outliers within the new data predicted from the multiple output chemistry model and acicular ferrite model were not removed because in a real situation no measured values would be there for comparison. In order to predict the weld metal toughness a neural network architecture was set up as defined in section 7.3, although the primary ferrite (PF) input was removed as has been previously discussed. The test temperature and weld metal toughness data could be linked to each appropriate data set, because the identification of the predicted data was known thus increasing the data quantity from 99 up to 485.

Training of the neural network using the predicted values for chemistry and AF% showed a degree of overfitting, as seen in Figure 7.28, in which the training error decreases with increased complexity up to a finite limit, and instead the test error is seen to increase. The optimum neural network model contained 11 hidden units, identified through examination of training and test errors and the predictions made by each respective modelling architecture. The predictions made on validation data can be seen in Figure 7.29, in which they are compared with predictions made using the weld metal toughness model described in section 7.3.1 utilising measured values.

Figure 7.28 – Average sum squared error compared with increasing complexity of the neural network model for weld metal toughness, utilising predicted values for weld metal chemistry and acicular ferrite content.
Figure 7.29 – Predictions of the weld metal toughness, comparing the use of predicted and measured values for weld metal chemistry and acicular ferrite content. The model using measured points contained 7 hidden units, whereas the model using predicted points contained 11 hidden units.

The predicted points in Figure 7.29 for measured and predicted input are not exactly a direct comparison because the model using measured values of chemistry and microstructure contained an added input for weld metal primary ferrite content. However, the primary ferrite content was seen to carry a relatively insignificant weighting, and therefore the models are theoretically similar showing a good correlation is seen in Figure 7.29. Obviously the predictions using measured values are seen to fit the ‘y=x’ ideal line the best in Figure 7.29, but the predictions made using previously predicted inputs fit far better than expected. Outliers are seen to carry far larger error bars on the points made using predicted input than those made using measured inputs, though this would be expected considering the relatively imprecise data, seen in Figure 7.27.

An investigation of the weightings placed on input to output connections and input to hidden layer connections, shown in Figure 7.30 (a) and (b) respectively, showed surprisingly close comparisons to those of the measured values, shown in Figure 7.5 (a) and (b). As with the modelling in section 7.3.1, seen in figure 7.5 (a) and (b), the input weightings in Figure 7.30 (a) and (b) show both test temperature and acicular ferrite content to carry the highest weightings with residual weightings placed on the weld metal chemistry parameters. The input weightings
show that predictions made using the weld metal toughness model utilising predicted values for weld metal chemistry and acicular ferrite carry a high level of confidence.

**Figure 7.30 (a)** – Input to output weights for a neural network model for weld metal toughness, containing 11 hidden units, utilising predicted values for weld metal chemistry and acicular ferrite content.
Figure 7.30 (b) – Input to hidden layer weights for a neural network model for weld metal toughness, containing 11 hidden units, utilising predicted values for weld metal chemistry and acicular ferrite content.

7.7 Discussion of the modelling of weld metal toughness using neural network techniques

Modelling of the weld metal toughness has been undertaken considering the many different contributing factors within the welding process, alloying elements and the eventual weld form. It has been found that the relevance placed on the various input parameters changes in relation to the values used at the input layer of the various modelling approaches. In order to evaluate the performance of a particular model it is not only essential to ascertain that the errors in training and testing are low and the predictions compared with actual values fit the ‘y=x’ ideal line closely, but the relevance weightings placed on individual inputs must fit with what is expected from metallurgical theory in order to be truly robust.

Throughout the modelling of weld metal toughness the test temperature, has been used as a flag to enable the repetition of all other input variables. As the test temperature is therefore a key parameter to the structure of the data available it is expected that this parameter would appear to
have the highest level of influence on the modelling. Relevance values for the test temperature have in general been seen to carry the highest weighting on input to output connections.

Of additional importance in the validation of the modelling is the relevance placed on other input variables. From the two main approaches to the modelling of weld metal toughness considered the most successful utilised microstructure parameters as inputs, however, clearly this information is not available from a manufacturing environment. It has been shown that a committee of models can be employed instead to obtain the necessary data values. Microstructure is an obvious choice when modelling the mechanical properties of a steel; in order to obtain optimum mechanical properties of the weld metal it is desirable to achieve a high volume fraction of acicular ferrite. Toughness predictions described in section 7.3 utilised the content of acicular ferrite (AF) and primary ferrite (PF), the two main constituents of the examined welds, along with weld metal chemistry values. Inclusion of the weld metal microstructure removes the need for any welding process parameters such as heat input and cooling of the weld metal. The acicular ferrite content is therefore expected to contribute strongly to the formation of rules around the data, and across the input to hidden layer connections this is indeed the case, shown in Figure 7.5 (b), with smaller weightings placed on weld wt.% aluminium (Al), oxygen (O) and nitrogen (N).

Oxygen is usually found in the form of oxide inclusions, which can have a detrimental effect on the weld metal toughness where a constant microstructure is present. All the welds in question did indeed contain a high volume fraction of acicular ferrite with smaller quantities of primary ferrite and other constituents. The high influence of oxygen was also seen in the neural network modelling of steel welds carried out by Lalam et al.\textsuperscript{99}, although the acicular ferrite content of the weld metal shows lower weighting in their work. The weighting of Al content is of no surprise, as this was seen to be present in inclusions as with oxygen; alumina (Al$_2$O$_3$) and the spinel galaxite (MnOAl$_2$O$_3$) were all found in the work outlined in Chapter 3. It is surprising however that if Al content is showing in such a way that the manganese (Mn) content is weighted so low. The neural network modelling technique employed is considered as a ‘blind’ method, forming rules around the data without prior knowledge of the quantities being considered. It is therefore possible to say that the data distribution of the Al data has been favoured over that of Mn in the formation of the rules around the training data. Embrittlement of the weld metal is caused by the presence of nitrogen, the exact mechanism is not clear, though a rule of thumb is that above 100ppm is unacceptable.
With the removal of the microstructure input parameters and addition of a more complex combination of process parameters and weld bead shape descriptors the change in influence yielded more interesting results. In Figure 7.8 (a) and (b) the microstructure parameters have been removed, and it was then shown that sulphur (S), carbon (C) along with nitrogen and oxygen were the most important factors. Sulphur is classed as an impurity along with nitrogen and phosphorous (P) contributing to lowering fracture toughness in steels. Once again impurities show high influence when looking across the weighting in the input to hidden layer, with C content of the steel also showing strong influence. Carbon content is a readily recognisable characteristic of the brittleness of steels; increasing the level of C in a steel leads to a decrease in the ductility, and hence a decrease in the weld metal toughness and would of course greatly influence the microstructure. A similar pattern was seen with the influence resting on the impurities and inclusion forming elements throughout development of the modelling, although the predictions made did not completely match that of the model outlined in section 7.3.

Various combinations of welding process parameters and weld bead shape descriptors were added in conjunction with the weld metal chemistry inputs in an effort to try and simulate the relationship between welding process and the eventual weld metal characteristics; namely the acicular ferrite content key to predicting the weld metal toughness successfully. The use of weld bead area was seen to act in a detrimental manner to the results when used in conjunction with other weld bead shape descriptors, as seen in Figure 7.22 and 7.23 (a) and (b). The closest results, as far as predicting weld metal toughness is concerned, compared with the model in section 7.3 was found to contain the complex number of inputs described in section 7.5.3. Predictions using the model from section 7.5.3 omitting the weld bead area, shown in Figure 7.23 (b) fit the ‘y=x’ as well, if not better than, those predictions made on validation data by the model described in section 7.3, with outliers appearing in a small quantity at the extremes of the data distribution.

It is obvious from the results obtained from the various approaches to the modelling of weld metal toughness through neural network techniques that the more complex the relationship between inputs and outputs the lower the accuracy of the results obtained will be. In the case of the acicular ferrite input, it was necessary to replace this single input with several inputs regarding heat input, welder speed, plate thickness and weld bead shape to determine the thermal cycle responsible for the formation of the microstructure. Swapping several inputs for a single input in order to gain the same level of results shows how difficult the problem is to model weld
metal toughness from welding process parameters, although a good level of confidence has been shown from the results obtained. It has also been shown that the use of a committee of neural networks, feeding outputs into the input layer of a neural network for weld metal toughness, can achieve similar levels of accuracy to those models utilising measured values. The work described in section 7.7 shows that weld metal toughness can be predicted from only the process parameters using a committee of neural networks to a high level of confidence, with the weightings placed on the input connections showing that the rules formed around the data correlated well with both expectation and those models trained using measured data inputs.
7.8 Weld Metal Hardness

The hardness of a material is a measure of a materials resistance to localised plastic deformation, for example a scratch or small indent. Various qualitative and quantitative methods are available to determine hardness, but all the data used in this chapter utilised the Vickers hardness test scale for a 5 kg load. Hardness measurements are taken at the ID, OD and mid-point of the two welds at 1 mm spacings from the centre-line (CL), as shown in Figure 7.31, also known as shell-sole-pit hardness testing. In order to determine hard spots, and therefore quantify the “true” hardness of the weld metal, further rows of hardness measurements are taken at 2 mm intervals across the weld metal from the ID to the mid-point, in the region of shading in Figure 7.31. This true hardness value, derived from an average of all the measurements described, is used for prediction purposes due to the quantity of data available.

![Figure 7.31](image)

Figure 7.31 – Specification for shell-sole-pit hardness measuring on multi-wire single pass per side line-pipe welds.

7.8.1 Initial approach to neural network modelling of weld metal hardness

Once data for the true hardness of the weld metal were collected and pre-processing was undertaken, a total of 181 data were obtained. In order to obtain the maximum data quantity, a 14 input architecture was used, utilising the following input variables:
Modelling of weld metal mechanical properties using neural network techniques

- Plate Thickness
- Welder Speed
- Heat Input
- Weld Metal wt.% Al
- Weld Metal wt.% Ti
- Weld Metal wt.% P
- Weld Metal wt.% S
- Weld Metal wt.% N
- Weld Metal wt.% O
- Weld Metal wt.% C
- Weld Metal wt.% Mn
- Weld Metal wt.% Mo
- Weld Metal wt.% Si
- Weld Metal wt.% \( \text{Si} \)
- ID or OD run

This 14 input architecture was trained, using the number of hidden nodes as the evaluating variable; training the neural network using 82 data, testing with 82 data and holding back 17 data for validation purposes. Training and test errors, shown in Figure 7.32, were seen to be relatively low; the relationship model complexity and training and test error is seen to be flat. Examination of predictions made using models of different hidden architecture enabled the determination of the optimum neural network model to contain 13 hidden units, though further investigation showed that the model produced poor results, Figure 7.33. This graph highlights the poor generalisation showing that the predictions made at the extremities of the data domain are made using rules fitting the data at the middle of the data domain better.

![Figure 7.32](image-url)  
Figure 7.32 – Average sum squared error for increased complexity of a 14 input neural network model for the prediction of weld metal hardness.
Figure 7.33 – Comparison of predicted points made using validation data against actual data for a 14 input neural network model, containing 13 hidden units, for weld metal hardness.

An investigation of the perceived significance values, $\sigma_w$, highlighted the input parameters that the model was using to form rules around the data for weld metal hardness. The input to output $\sigma_w$ values and input to hidden layer values are shown in Figure 7.34 (a) and (b) respectively, and these results show that little weighting is placed on both the weld metal carbon content or the welding process heat input important parameters in the formation of a hardened weld metal. In order to improve the model, the information gathered through investigation of the perceived significance enabled the removal of certain input parameters carrying low weighting with respect to the modelling of weld metal hardness. The input parameters removed were; heat input, weld metal wt.% C and weld metal wt.% Mn. This is perhaps surprising because clearly C in particular is expected to alter the hardness of a weld significantly. Due to the nature of neural networks, classed as a blind technique, issues with regard the data patterns present may dominate scientific principles within the data, and therefore modelling without certain theoretically important parameters was undertaken for interest.
Figure 7.34 (a) – Perceived significance values for input to output layer connections for a 14 input neural network model, containing 13 hidden units, modelling weld metal hardness values

Figure 7.34 (b) – Perceived significance values for input to hidden layer connections for a 14 input neural network model, containing 13 hidden units, modelling weld metal hardness values
7.8.2 Evolution of the neural network model for weld metal hardness

The same pre-processing and data quantities were used as described in section 7.8.1, utilising an 11 input architecture, and varying the number of nodes in the hidden layer as an evaluating parameter. The errors on training and testing, shown in Figure 7.35, were seen to have improved, with training error now of the order of $5 \times 10^{-3}$ compared with training error for the model in section 7.8.1 being approximately 0.01. This improvement was clearly evident in the predictions made when compared with actual data on training, test and validation data, utilising the optimum neural network architecture containing 7 hidden units, seen in Figure 7.36. The predictions made using the 7 hidden unit neural network architecture seen in Figure 7.36 fit the ‘$y=x$’ ideal line far better than the predictions found in Figure 7.33.

![Figure 7.35](image_url)  

**Figure 7.35** – Average sum squared error for increased complexity of an 11 input neural network model for weld metal hardness
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Figure 7.36 – Comparison of predicted points made using validation data against actual data for a 11 input neural network model, containing 7 hidden units, for weld metal hardness.

An evaluation of the perceived significance, $\sigma_w$, values associated with the modelling of weld metal hardness using the reduced number of inputs enables the level of confidence in predicting weld metal hardness to be identified. The $\sigma_w$ values across both input to output layer and input to hidden layer, shown in Figure 7.37 (a) and (b) respectively did not place any influence on any single parameter in particular. Across input to output connections, the weld metal nitrogen, titanium and molybdenum along with the welder speed held highest influence upon the output of the model, whereas, across input to hidden layer connections weld metal molybdenum, sulphur and oxygen along with welder speed and plate thickness showed highest relative influence.
Figure 7.37 (a) – Perceived significance values for input to output layer connections for an 11 input neural network model, containing 7 hidden units, modelling weld metal hardness values.

Figure 7.37 (b) – Perceived significance values for input to hidden layer connections for an 11 input neural network model, containing 7 hidden units, modelling weld metal hardness values.
7.8.3 Discussion of the modelling of weld metal hardness

Variations in hardness across the weld metal are seen due to the thermal cycle experienced at various points within the weld metal, especially where a second weld run overlays an initial run, as in the case of the ID and OD welding of line-pipe leading to hard spots due to re-heating. It is also important to take into consideration the chemical composition and microstructure of the weld metal, with concentrations of carbon and nitrogen causing localised hardness increases.

When modelling the hardness, or any other mechanical property of the weld metal, it is important to take into account the microstructure, chemical composition and any tempering effects; these parameters are in turn influenced by the welding conditions and thermal cycle. Bhadeshia puts forward this case in his review of modelling mechanical properties of steel welds, identifying the key to successful modelling as determination of the microstructure within the steel. When utilising so-called blind modelling techniques, it is also important to ensure that such all contributory factors are considered in the modelling algorithm. In the case of the modelling presented in this section, it was found that inclusion of the weld metal would not allow for the maximum quantity of data to be obtained. However, welding process parameters have a complex and remote relationship to the microstructure have been included here. The strong ability of neural networks to identify hidden patterns within the data, such as the relationship between welding conditions and the weld metal hardness, allows for information having a complex relationship with the output to be utilised, presenting a strong case for their use here.

Two modelling architectures were assessed, the second evolving from information gained from initial models; the first model showed relatively poor results while the second showed a good correlation with the ‘y=x’ ideal line. The approach to modelling hardness followed a simplified view of the welding process, as was seen to work well in the modelling of weld metal toughness, using a measured heat input calculated from the values for amps and volts on each welding wire. Perceived significance values, \( \sigma_w \), across the input to output layer connections showed the chemical additions molybdenum (Mo), silicon (Si) and oxygen (O) to carry relatively high weightings, with all over chemical input parameters carrying similar weightings apart from those for weld metal C and Mn having relatively insignificant weighting. Welder speed is seen to have a relatively high level of influence, though other welding condition parameters carry relatively
low weightings. These findings are surprising, as it is expected that the major influence would be placed upon the heat input to the welding system along with the weld metal content of C and Mn, both being present in relatively high concentrations and being responsible for the mechanical properties of the weld metal, through promotion of inclusions, microstructure refinement and embrittlement of the material.

Assessment of the $\sigma_w$ values across the input to hidden layer connections gave no insight into the weightings placed on parameters, with the weld metal titanium (Ti) content carrying a majority of the weighting followed by weld metal O content. All other input parameters show insignificant weightings across the input to hidden layer connections. Of the welding process inputs, plate thickness is seen to carry greatest weighting, though small compared to weld metal Ti, meaning that it would be kept as an input for the evolved model. Even though the $\sigma_w$ values showed results that did not match what was expected from metallurgical principles, it was decided to remove the three input parameters found to carry least influence; heat input, weld metal C, and weld metal Mn. This removal of theoretically key parameters was done as issues relating to the distribution of data for these inputs may have been the cause of the lack of influence, therefore modelling without them should show an improvement if this is so.

The evolutionary step, removing key parameters, showed an improvement in the predictions made using an optimum trained neural network, as seen in Figure 7.36 compared with Figure 7.33. This would not be expected if the problem were looked at from a physical principles stance, though it was expected due to the distribution of data used in this modelling. Perceived significance values across the input to output connections highlighted weld metal N, T and Mo as having a significant weighting on the weld metal hardness. Welder speed is also seen to play a strong role in the relationship with weld metal hardness, contributing a strong influence over the thermal cycle at the weld. Across the connections between input layer and hidden layer, nitrogen content is seen to lose its role as an influential parameter, with the weightings being mainly placed on weld metal Mo, S and O along with the process parameters welder speed and plate thickness.

A good correlation has been achieved with the 'y=x' ideal when modelling the weld metal hardness using neural network techniques. Although a relatively small quantity has been used in training and testing, the predictions made have shown very little error across the full data domain.
available. Removal of certain parameters resulted in significant improvement, when compared to the initial modelling of weld metal toughness. It is proposed that given more quality data, and inclusion of certain key parameters such as the microstructure of the weld metal even better results can be achieved.
7.9 Weld Metal UTS

Following yielding of a material, the stress necessary to continue plastic deformation in metals increases to a maximum. The ultimate tensile strength (UTS) is the stress at the maximum on the engineering stress-strain curve for a given material, an example of the stress-strain curve for steel is shown in Figure 7.38. The peak stress responds to the maximum stress that can be sustained by a structure in tension; if this stress is applied and maintained, fracture will result. The tensile strength is expressed as either megapascals (MPa), meganewtons per metre$^2$ (MN/m$^2$) or newtons per millimetre$^2$ (N/mm$^2$). The range of UTS values modelled in this section was from 595 to 722 N/m$^2$ with mainly all the data being taken from OD welds.

![Stress-strain curve for mild steel showing yield point (Y), ultimate stress (Z), also known as the UTS, and breaking point (W).](image)

**Figure 7.38** – Stress-strain curve for mild steel showing yield point (Y), ultimate stress (Z), also known as the UTS, and breaking point (W).

7.9.1 Initial modelling of weld metal UTS

A similar approach to the modelling of weld metal hardness, described in section 7.8, was used to develop an accurate model for the weld metal UTS. Pre-processing produced only 61 data, giving the same 14 input parameters as weld metal hardness for this optimum data quantity. The small data volume meant that the data were divided into 31 training data and 30 test data, and omitting validation data. The 14 input architecture was trained, using the number of nodes in the
hidden layer as the evaluative variable. Error in training and testing for increased complexity of the neural network architecture are seen in Figure 7.39, with the training error being of the order of magnitude of $7 \times 10^{-3}$ without any related overfitting seen in the test data. The optimum neural network model is seen to contain 7 hidden units, and predictions compared with the actual data are shown in Figure 7.40 following the ‘$y=x$’ ideal line closely.

![Figure 7.39 - Average sum squared error for increased complexity of a 14 input neural network model for weld metal UTS](image)

**Figure 7.39** - Average sum squared error for increased complexity of a 14 input neural network model for weld metal UTS

![Figure 7.40 - Comparison of predicted points, made using validation data, against actual data for a 14 input neural network model, containing 7 hidden units, for weld metal UTS](image)

**Figure 7.40** - Comparison of predicted points, made using validation data, against actual data for a 14 input neural network model, containing 7 hidden units, for weld metal UTS.
A good correlation between actual data and predicted points is observed in Figure 7.40, although in order to determine the level of confidence at which predictions can be made the perceived significance values, $\sigma_w$, were assessed to identify the input parameters that the neural network is using to form the rules around the data. The $\sigma_w$ for connections across input to output layer and input to hidden layer are shown in Figure 7.41 (a) and (b) respectively.

**Figure 7.41 (a)** – Perceived significance values for input to output layer connections for a 14 input neural network model, containing 7 hidden units, modelling weld metal UTS
The input parameters for weld metal Mn and Mo dominate the algorithm for weld metal UTS, when considering the connections between input and output layer, shown in Figure 7.41 (a), while very little relevance is placed on any other inputs. Across the input to hidden layer connections, seen in Figure 7.41 (b), weld metal Mn loses its high weighting, with the distribution of influence being placed on weld metal S, C, Mo, plate thickness and heat input. Insignificant relevance ratings are seen for weld metal Al, Ti, N and O across both input to output connections and input to hidden layer connections.

7.9.2 Development of the neural network model for weld metal UTS

The development of the model for weld metal UTS followed the same strategy of hardness model, removing 3 input parameters as in section 7.8. Of the four input parameters identified as carrying relatively insignificant relevance in section 7.9.1 for the initial UTS model the weld metal Al, N and O were removed, leaving in the weld metal Ti content as an input parameter even though low weighting was seen to be placed on it. Pre-processing was carried out as previously, with the same quantities of data being made available to training and testing as in section 7.9.1.
Training and testing yielded the error values shown in Figure 7.42 for increasing complexity of the neural network architecture. The optimum architecture was seen to contain 7 nodes in the hidden layer, although training and test error carried no significant gain over the initial modelling of UTS in section 7.9.1. Predictions using this 7 hidden unit architecture, compared with actual data shown in Figure 7.43 also showed no significant gain in performance over the model in section 7.9.1. The only perceived gain at this stage would be the need for less input parameters, while still gaining the same level of performance in predictions.

Figure 7.42 - Average sum squared error for increased complexity of an 11 input neural network model for weld metal UTS
Figure 7.43 - Comparison of predicted points, made using validation data, against actual data for an 11 input neural network model, containing 7 hidden units, for weld metal UTS.

Perceived significance values, $\sigma_w$, were examined in order to identify if the model was performing to a level of confidence matching to expectations of prior metallurgical knowledge. The $\sigma_w$ values across input to output layers, and input to hidden layer are shown in Figure 7.44 (a) and (b) respectively.
Figure 7.44 (a) – Perceived significance values for input to output layer connections for an 11 input neural network model, containing 7 hidden units, modelling weld metal UTS

Figure 7.44 (b) – Perceived significance values for input to output layer connections for an 11 input neural network model, containing 7 hidden units, modelling weld metal UTS
7.9.3 Discussion of the results of neural network modelling of weld metal UTS

Throughout the literature many attempts at modelling the weld metal yield and ultimate tensile strength using neural network techniques have been made, although the majority of work is concerned with single bead and single wire welding. Lalam et al. used a greater number of weld metal chemical elements in their modelling of weld metal toughness, along with more detail as to initial welding heat input and any tempering or interpass temperatures. The welding considered in this chapter were one pass per side, with the majority of UTS results being taken from OD welds, therefore post weld heat treatment (PWHT) is not an issue here. The modelling of UTS of Yurioka et al. uses similar inputs to those described in this section, though the predictions made in their work fit the ‘y=x’ ideal much closer. The larger error in the prediction in the work of this section are explained by the much smaller quantity of data used in modelling, not enabling the model to train on a sufficient distribution of examples and therefore not generalising as well as that found in the results of Yurioka et al. Models have also been presented that utilise the input of the yield strength (YS) in the prediction of UTS. The aim of the work presented in this section is to develop a suitable neural network model to determine the weld metal toughness for multiple wire, submerged arc welds identifying the ID and OD weld metal toughness values using input parameters readily available from the welding process.

Modelling inputs chosen were the same as those for the modelling of weld metal hardness, due to the same problems encountered previously in obtaining the maximum data; this also meant that key parameters such as microstructure were omitted from the modelling. In physical modelling of weld metal mechanical properties theories have been put forward as to the non-linear relationship between weld metal hardness and the weld metal UTS. Evolution of the models defined where the differences in modelling weld metal hardness and UTS were to be found; hence the inputs removed were different through assessment of the perceived significance values indicative of the rules formed around the data by each model. No significant improvement in the average sums squared error values was seen across the full range of model complexity for either the 14 input models, shown in Figure 7.39, or the 11 input models, shown in Figure 7.42. The insignificant improvements are also reflected in the predictions made across the training and test data domains; the lack of improvement can be attributed to the small amount of data used in training the neural network. The low quantity of data used in training yielded good results, though this high level of performance would only apply to data prediction over the small data domain considered in training.
Examination of the perceived significance values, $\sigma_w$, showed differing results for the 14 input and 11 inputs models; explained by the need for re-distribution of the weightings where inputs parameters are reduced. Key input parameters were found to be weld metal wt.% Mn, Mo, C, S, plate thickness and heat input with some residual weighting on other input parameters in the 14 input neural network model. When the number of input parameters is reduced the relevance weighting is placed on weld metal wt.% Mn and plate thickness with insignificant relevance placed on all other parameters; showing a bad formation of rules around the data. From the results of input relevance on both 14 input and 11 input models, the most robust model is determined to have 14 inputs due to the formation of the rules around the data fitting prior metallurgical expectation far better.
7.10 Conclusions

- Successful neural network models have been developed for the modelling of weld metal toughness characteristics, weld metal true hardness and weld metal UTS from weld process inputs for OD welds.

- Modelling of weld metal toughness has been successfully achieved using neural network techniques contemplating weld metal chemistry and weld metal microstructure constituents for OD welds. It has also been possible to predict weld metal toughness using neural network techniques considering weld metal chemistry, simple welding process parameters and weld bead shape descriptors for OD welds.

- The temperature at which the weld metal toughness has been determined as a key parameter in this modelling; firstly due to the structuring of the weld data and secondly due to the intrinsic relationship between the temperature and the ductility of the steel.

- The acicular ferrite content has been found to be a key parameter to the modelling of weld metal toughness, independent of the data structure. Acicular ferrite is not a readily available parameter, and therefore modelling inputs must be included that represent this microstructural factor.

- Modelling of the weld metal toughness using detailed combinations of the welding process inputs yielded poor results compared to simplified inputs, for example using heat input in place of the specific voltage and current on each individual welding wire.

- Inclusion of the weld bead area when compared to describing the weld using a variety of measurements; namely cap height, bead penetration, weld width and flare region, yields poor results. The use of describing measurements give more detail as to the shape of the area; therefore relating to the cooling rate and formation of microstructure far better.

- Comparative results to the modelling of weld metal toughness utilising weld metal chemistry and microstructure were achieved using the following input parameters; plate thickness, welder speed, measured heat input, weld metal wt.% C, Mn, Si, Al, P, S, N, O,
test temperature, cap height, weld width, bead penetration and flare region measurements. Indicating that a good combination of parameters have been utilised, representing all contributing factors attributable to the weld metal toughness and acicular ferrite content.

- Predicted results of weld metal chemistry and weld metal acicular ferrite content have been successfully utilised in the neural network modelling of weld metal toughness. Results of modelling with predicted inputs showed comparative accuracy with modelling using measured inputs, for the same input architecture.

- A neural network model has been successfully trained to predict weld metal true hardness utilising plate thickness, welder speed, weld metal wt.% Mo, Si, Al, Ti, P, S, N and O and a binary flag to identify the ID or OD run. The smaller quantity of data available to the modelling of weld metal hardness compared with weld metal toughness has shown that the rules formed around the data omit certain important metallurgical factors; these being heat input weld metal wt.% C and Mn.

- A successful model for the weld metal UTS has been developed using neural network techniques, though this has been trained using a very small quantity of data. The small quantity of data used in training therefore limits the domain of accuracy for this particular model. No improvements were seen when reducing the number of inputs for the UTS model, explained by the small data quantity available.

- Modelling of weld metal mechanical properties has been shown to be possible, using welding process parameters and information regarding welding consumables. The use of committee’s of neural networks to obtain data not readily predicted from manufacturing information overcomes the problems related to key inputs not available at the production level. It is proposed that the principles here are easily applied to all weld metal characteristics provided sufficient data is available.
7.11 Chapter Summary

In order to reduce the cost of any commercially produced weld it is important to ascertain the optimum manufacturing method with little outlay on experimental testing. Welding engineers presently determine the best method using skills and knowledge accumulated through experience gained through years of costly, time consuming experimental trials. Any attempt to simplify this methodology through quantitative modelling must recognise the complex nature of the weld metal and processes involved. Ideally modelling should be based on firm physical principles that once established can be used with greater confidence and are capable of predicting new phenomena, although this can become overwhelming with many phenomena interacting and influencing the many characteristics of weld metal.

Blind procedures such as regression analysis and neural networks can reveal new regularities in the data by closely mimicking human experience through learning or being able to recognise correct science. In this chapter neural network techniques have been applied to the complex relationships between the welding process inputs and the weld metal mechanical properties; namely weld metal toughness, weld metal true hardness and weld metal UTS. The main work within this chapter has been concerned with the modelling of weld metal toughness due to the need for a good quantity of quality data for the training of the neural network models for the complex relationships being considered. Impact testing is undertaken at different temperatures, and therefore it was possible to use these temperature values as flags allowing repetition of other information for each weld concerned at each test temperature. The use of smaller quantities of data, found in the work related to modelling weld metal hardness and UTS, although showing good correlation with the ‘y=x’ ideal showed weightings placed on parameters that would not be expected from a physical modelling perspective. The weightings placed on the models for hardness and UTS indicate that the models are therefore only valid across the particular data domain being presented to the neural network.

Various approaches were taken to the modelling of weld metal mechanical properties utilising weld process inputs, weld metal chemistry, weld microstructure and weld geometry. Evaluation of the contribution of all the various inputs, contemplating complex and simple input architectures to describe the same thing; for example heat input compared with the use of the voltage and current applied to the individual wires. It was found that modelling using weld metal chemistry and microstructure, removed the need for plate, and wire chemistry and process
variables, yielded the best results however, this information is not readily available from the welding process. As the object of the modelling was to obtain a modelling architecture utilising information easily available from a manufacturing standpoint, a more complex model was needed to obtain similar results. Various modelling architectures were assessed, with an input architecture contemplating simple welding process parameters, weld metal chemistry and measurements describing weld cap, bead penetration, weld width and flare region. I was possible to produce results comparable to the modelling using weld metal chemistry and microstructure.

Modelling of the weld metal toughness has also been undertaken utilising a committee of neural networks. The use of a committee enabled the prediction of key parameters vital for accurate prediction of the weld metal toughness. The first layer of neural networks was used to predict weld metal chemistry and acicular ferrite content from known parameters, before feeding the predictions as inputs to the weld metal toughness model. The results from the use of predictions showed excellent correlation with the \( y=x \) ideal, with very few outliers when compared to similar modelling utilising measured values as inputs.

A simpler modelling approach was undertaken with regards the weld metal hardness and weld metal UTS, mainly due to the smaller amounts of data available. Developments of the models enabled the determination of the most robust model to be used. The examination of the weighting placed on the various inputs showed that the rules formed around the data did not follow what would be expected from prior metallurgical knowledge, though this was expected to a degree due to the small quantities of data being examined.

The work in this chapter has shown that for complex modelling relationships, such as the determination of weld metal mechanical properties, neural networks are a valuable tool. The use of such blind modelling techniques allow for the reduction in the amount of modelling effort related to the overwhelmingly complex nature of the characteristics of weld metal with respect to the welding process inputs. The models presented in this chapter have shown that a range of mechanical properties can be accurately predicted from welding process parameters and consumable chemistries, utilising a variety of techniques fully exploiting the potential of neural network modelling.
Chapter 8 – Application of modelling techniques to the ID weld metal

8.1 Introduction

In the submerged arc welding of line-pipe two separate welding runs are utilised to obtain the optimum join for the thick plate. A multi-wire system with a close spacing between weld electrodes prevents individual solidification of weld deposits from each wire in a particular run, removing any detrimental effects of re-heating. In order to obtain good weld penetration the plate edges are machined prior to welding which also influences the final weld shape. The angle and depth of the preparation at the inner diameter (ID) and the outer diameter (OD) have an important role to play, especially where the ID weld is concerned. The weld preparation is, a defining factor in the heat sink available to the ID welding process and strongly defines the eventual weld bead shape. The preparation of the plate and selection of appropriate welding procedures is typically undertaken through exhaustive trials, which are costly and time consuming.

In order to model any characteristic of a submerged arc weld from line-pipe a very complex two stage welding process must be considered involving the plate preparation, plate chemistry, consumable chemistry, welding process parameters and the eventual weld metal microstructure formed. The microstructure of the weld metal is strongly defined by the cooling procedure. Consideration of the contributing parameters is made more complex for ID welding, as further inputs are required to identify the contributing factors from the OD preparation, as defined in Figure 8.1, when compared to OD modelling. Previously in chapters 5, 6 and 7 the OD model assumed that the ID weld fully filled the preparation of the parent plate, and therefore only the plate thickness and OD preparation were needed to model the OD welding process.

This chapter applies the modelling strategies for weld metal mechanical properties, microstructure and geometry developed in earlier chapters for OD welding, whilst taking into account the different preparation geometry experienced during welding of the ID and any re-heating which takes place during the OD welding process. The main thrust of the chapter develops the previous work on prediction of OD weld bead shape to the entire weld, i.e. including the ID weld. A model for the entire weld bead shape is extremely useful for the development of a through process model, in which weld bead shape is a desired input.
Application of modelling techniques to the ID weld metal

Figure 8.1 – Identification of the parent plate preparation for the single pass per side multi-wire submerged arc welding of line-pipe.

8.2 The modelling of ID weld bead shape

In order to consider the visible shape of the ID weld after welding is complete and determine the relative position in comparison to the OD bead a two-model process was adopted. The visible ID bead, seen in Figure 8.1, is the shape of the ID weld that can be measured which is not covered by the overlaid OD weld. Measurements were taken at 30° intervals from 0° to 150° and 210° to 330° to give an 11-output architecture describing the visible ID weld bead. In order to predict the relative position of the ID bead with respect to the OD bead, a second neural network was then developed to predict the distance from ID origin to OD origin, the OD penetration and the point of contact of the OD and ID weld bead edges, as defined in Figure 8.2.
Application of modelling techniques to the ID weld metal

![Diagram of ID and OD welds with parameters](image)

**Figure 8.2** – Measurements used in modelling the position of the ID weld bead shape in relation to the OD weld bead.

### 8.2.1 Modelling of the visible ID weld bead shape

It was necessary to have a greater number of inputs for the modelling of ID, due to the need for information about both the ID and OD plate preparation, with a total of 19 input parameters being used. The number of outputs was also affected because the penetration measured at 180° was not visible, and therefore only 11 outputs were modelled, compared with 12 in chapter 6. The inputs for modelling the visible ID weld were as follows:

**Inputs:**

- Plate Thickness
- ID Preparation Angle
- ID Preparation Depth
- OD Preparation Angle
- OD Preparation Depth
- Preparation Nose
- ID Amps – Wire 1, 2, and 3
- ID Volts – Wire 1, 2 and 3
- ID Wire Angle – Wire 1, 2 and 3
- ID Welder Travel Speed
- ID Vertical Stickout
- ID Spacing wire 1 → 2, 2 → 3

The data were pre-processed as carried out in chapter 6 involving normalising between the limits 0.5 to –0.5, randomising and splitting into training and testing data sets. A total of 162 data were available following pre-processing; 81 data were allocated to training and 81 to testing. The validation data set was omitted due to the small quantity of data available. Training was
undertaken with a constant number of nodes at the input and output, with a varying number of nodes in the hidden layer, used as the evaluative variable.

It is shown in, Figure 8.3, that the test error increased as the training error decreased. This trend in training and test error was also observed in previous work on OD weld bead shape. The increasing test error makes evaluation of the optimum modelling architecture difficult. It is therefore necessary to evaluate the predicted data from each model by comparing with the measured target values. It was found from an examination of the predictions made, as a function of increasing complexity, that the optimum neural network model for visible ID shape contained 9 hidden units. Predictions of each individual measurement around the weld, made using both training and test data, were shuffled and combined to form a validation data set, as shown in Figure 8.4 (a)-(k).

From the information in Figure 8.4 it can be seen that the predictions compared with actual data follow the 'y=x' ideal line and it is possible to identify the trends in weld bead geometry. The highest degree of error is seen at 150° and 210° which are at the edges of the data set.

Figure 8.3 - Average sum squared error with increasing complexity of the neural network model for visible ID weld bead shape

In order to evaluate whether or not the model is forming rules around the data correctly in the modelling of the ID weld bead shape the perceived significance values, $\sigma_w$, were examined to
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determine the influential input parameters. The $\sigma_w$ values across input to output connections and input to hidden layer connections are shown in Figure 8.5 (a) and (b) respectively.

From the $\sigma_w$ values across input to output connections, Figure 8.5 (a), it can be seen that the ID preparation depth carries the greatest influence on the modelling. This is perhaps to be expected as the weld preparation is machined with the purpose of generating good penetration and fill. The next ranked parameter is the angle of wire number 2, which influences the spread of the weld body, and therefore affects the width of the weld. All other parameters are seen to carry very little weighting in comparison to the main influential parameters, however, the OD preparation depth, OD preparation angle, spacing between wires 1 and 2 and wires 2 and 3, and the voltage across wire number 3 are all seen to carry small but significant weightings.

Across the connections between the input and hidden layer, seen in Figure 8.5 (b), the $\sigma_w$ values highlighted volts across wire 3 and wire 1, ID preparation depth and angle and the vertical stickout of the welding wires to carry greatest influence over the weld bead shape. The preparation of the plate is seen to play a significant role, as expected due to the machining undertaken to obtain the desired ID weld bead. The role of the voltage is explained through the presence of Lorentz forces causing stirring within the weld metal, forcing the weld metal to fill and spread into the parent plate. The vertical stickout of the welding wire is responsible for the deposition rate of the welding wires, heat input and the weld cap shape through altered rates of weld cooling and solidification of the molten pool$^{15}$. 
Figure 8.4 – Predicted points, made using training and testing data, compared with measured data for a neural network model for the visible ID weld bead shape. (a) distance at $0^\circ$ (b) distance at $30^\circ$ (c) distance at $60^\circ$ (d) distance at $90^\circ$ (e) distance at $120^\circ$ (f) distance at $150^\circ$. 
Figure 8.4 – Predicted points, made using training and testing data, compared with measured data for a neural network model for the visible ID weld bead shape. (g) distance at 210° (h) distance at 240° (i) distance at 270° (j) distance at 300° (k) distance at 330°.
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**Figure 8.5 (a)** - Perceived significance values, $\sigma_w$, across input to output connections for a model for visible ID weld bead shape containing 9 hidden units

**Figure 8.5 (b)** - Perceived significance values, $\sigma_w$, across input to hidden layer connections for a model for visible ID weld bead shape containing 9 hidden units
8.2.2 Prediction of positioning parameters for the visible ID weld bead shape in relation to the OD weld bead

The parameters described in Figure 8.2 were used in locating the visible ID weld bead in relation to the OD weld predictions described in chapter 6, enabling the prediction of the complete weld bead shape. Using the following inputs a 14 input model was developed to predict the OD penetration, distance from OD origin to ID origin and the two points at which the OD weld bead edge met the ID weld bead edge, i.e. where the OD bead overlays the ID, represented as a measurement and an angle from the OD origin.

Inputs:

- Plate Thickness
- ID Preparation Angle
- ID Preparation Depth
- Nose
- OD Preparation Angle
- OD Preparation Depth
- ID + OD Amps Wire 1
- ID + OD Volts Wire 1
- ID + OD Wire Angle - Wire 1
- ID + OD Welder Speed

Pre-processing was carried out, involving normalising between the limits -0.5 to 0.5, randomising and splitting the data in the ratio of 82 training data and 81 test data. Training was undertaken maintaining a constant number of inputs and outputs whilst increasing the number of nodes in the hidden layer as the evaluative variable. The errors in training and testing are seen in Figure 8.6, which shows a relatively high performance for a 4 output neural network model compared with previous multiple output modelling. Examination of the error values and predictions made using neural networks containing different numbers of nodes in the hidden layer found that the optimum model contained 9 hidden units. Predictions of the OD penetration and distance between the ID and OD origins are shown in Figure 8.7 (a), with predictions of the distance and angle of the two points of contact of the ID weld and OD weld edge from the OD origin shown in Figure 8.7 (b). All points were made using a validation data set made by re-shuffling and combining the training and test data.
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Figure 8.6 – Average sum squared error compared with increased complexity of a neural network model for positioning parameters for OD weld bead and visible ID weld bead.

Figure 8.7 (a) – Predicted points of the OD penetration and distance from ID to OD origin, made using validation data on a neural network model containing 9 hidden units, to be used for positioning the visible ID weld bead in relation to the OD weld bead.

Figure 8.7 (b) – Predicted points of the distance and angle of the two points of contact of the ID weld and OD weld edge from the OD origin, made using validation data on a neural network model containing 9 hidden units, to be used for positioning the visible ID weld bead in relation to the OD weld bead.
8.2.3 Combination of results to predict images of visible ID weld bead shape

In order to gain a visual appreciation of the predicted results, measured and predicted data were used to create images of three welds from the data. The chosen three welds were also used in chapter 6, therefore allowing the OD and ID images to be linked later in this chapter. Using the predicted points from the visible ID model, in section 8.2.1, and the points of contact between ID and OD weld, in section 8.2.2, the images in Figure 8.8 were created. In Figure 8.8 (a) – (c) the measured weld shape is drawn in the solid line, while the dashed line represents the predicted weld. Measurements taken at 150° and 210° are also shown, a black spot for measured and red spot for predicted value, these points correspond to a point on the overlying OD weld bead. The compared images show a good correlation between measured and predicted data in Figure 8.8. These predictions are comparable in accuracy to those for the OD presented in chapter 6 127.

8.2.4 Discussion of the modelling of ID weld bead shape

In a multi-wire welding scenario, it is imperative that the wires all feed in to the weld pool such that the weld pool solidifies as a single mass. It is clear that there are a number of factors contributing to the final weld bead shape, including electrode characteristics, plate geometry and weld process parameters. The dominant forces acting on the weld pool originate from the direction of movement of the welding head and a Lorentz force from the passage of the current through the liquid metal from each electrode. The complex relationship between welding parameters, consumables and parent plate with the final weld bead is discussed in great detail in chapter 6. Modelling of the ID weld bead shape requires the inclusion of yet more input parameters due to the nature of the two stage welding process for OD and ID welding. The thickness of the plate directly surrounding the welding region plays a strong role in influencing the final weld bead shape due to the heat sink factors linked to cooling. When welding of the ID is undertaken the OD preparation of the plate is present and therefore reduces the volume of adjacent material, thus reducing the heat sink.
Application of modelling techniques to the complete weld structure

Figure 8.8 - Predicted visible ID weld bead images compared with measured visible ID images from submerged arc welds of line pipe material, showing a variety of weld bead sizes. Predicted image drawn in dashed line, measured image drawn in solid line, predicted points on OD weld are red dots, measured points on OD weld are black dots. Images are not drawn to scale.
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From the modelling of visible ID weld bead geometry comparable results to those obtained from the work in chapter 6, considering OD weld bead geometry have been achieved. The examination of the input relevance's in the neural network models of bead shape are in excellent agreement with the experimental observations and have provided a useful insight, which concurs with metallurgical knowledge. The $\sigma_w$ values shown in Figure 8.5 (a) and (b) placed the strongest weightings on the ID preparation depth, ID preparation angle along with a varied response to parameters representing the wire angles, spacing and electrical settings to varying degree. It was also observed that across the input to hidden layer connections a relatively high influence is placed on the OD preparation depth and angle, as expected. Preparation of the parent plate is key to ensuring a sound join in thick walled line-pipe material, before forming the flat plate into an 'O' planing of the edges is undertaken to obtain the v-preparation used in the modelling work. Much work is found with regard to experimental trials and development of both plate preparation of welding procedure\textsuperscript{14,16,132}.

The presence of Lorentz forces caused by the passing of current through the molten pool are not only responsible for stirring of the liquid metal, but also play a vital role in applying forces responsible for the formation of the final weld bead alongside the driving force created from the welding speed. The forces applied on the molten weld metal influence the penetration, weld width and any flare that occurs in the weld geometry\textsuperscript{100}.

The modelling of weld bead ID has shown a good correlation with prior expectation with influence being placed on the various welding process parameters with varied weight. The key parameters expected to strongly sway the modelling of weld bead shape were those referring to both ID and OD plate preparation. The influence placed on the preparation parameters was relatively high, as seen in Figure 8.5 (a) and (b). With the increased complexity of the input layer due to the need for the OD and ID information it is clear from the $\sigma_w$ values that a robust model has been developed. With reference to the modelling of positioning parameters the results of error on training and testing were found to be excellent, although the relationship between OD penetration and distance between origin at OD and ID is relatively simple and good results are expected. The high level of confidence in the positioning model gives rise to the ability to combine the modelling of chapter 6, regarding OD weld bead geometry, and the visible ID weld geometry covered in this chapter, seen in the following section.
8.2.5 Combination of the Predicted OD Images and visible ID images

The ultimate aim of the work on predicting the visible ID weld bead shape was to be able to combine the outputs of the optimum model with the best model for OD weld bead shape, utilising the positioning model to create a complete image of a predicted line-pipe weld. The combined images can be seen in Figure 8.9, showing that a close match has been achieved between measured weld geometry, drawn in a solid line, compared with the image created using predicted points, drawn in the dashed line. Any rotation or misalignment between the central axis of both ID and OD welds is compensated for through the positioning model as is seen with the non parallel x axis of the ID in relation to the OD. The welds in Figure 8.9 (a) – (c) cover a variety of welding shapes and sizes found within the data used in modelling here. A relatively close correlation between measured images and predicted is seen in Figure 8.9 (a) – (c) considering the highly complex nature of the models developed.

![Figure 8.9](image)

**Figure 8.9** – Predicted images compared with measured geometry for both ID and OD welds for single pass per side multi-wire submerged arc welds from line-pipe. Predicted image drawn in dashed line, measured image drawn in solid line; images are not drawn to scale.
8.3 Neural network modelling of ID weld metal microstructure

During the two-stage process for welding line-pipe re-heating of the ID weld occurs as a consequence of the OD welding process. This leads to differing microstructure volume fractions between the ID and OD weld metal. The differences in microstructure can have highly influential effects on the weld metal properties, and therefore it is paramount that any detrimental effects can be determined. In the modelling of the weld metal microstructure content for the ID, it is important to take into account the heat input from the OD welding phase as well as the heat input initially applied during ID welding. Two models have been developed in this section, utilising techniques found in chapter 5 section 6, the first considers only acicular ferrite content, whereas the second use a multiple output approach to predict the acicular ferrite (AF), primary ferrite (PF) and ferrite side-plate (FS) content, the three major microstructure constituents found in the welds modelled here.

8.3.1 Approach to ID weld acicular ferrite content modelling

The approach to modelling the acicular ferrite content of the ID weld metal followed that for the OD, as described in chapter 5 section 6, although an extra input was added to represent the heat input of the OD welding process. Normalising between -0.5 and 0.5 was undertaken, followed by randomising and splitting to form 62 training data, and 62 test data a validation data set was omitted due to the small quantity of data available. Inputs used were; plate thickness, welder travel speed, ID heat input, OD heat input, weld metal wt.% carbon (C), manganese (Mn), chromium (Cr), molybdenum (Mo), silicon (Si), aluminium (Al), titanium (Ti), sulphur (S), nitrogen (N) and oxygen (O).

The errors in training and testing, shown in Figure 8.10, were seen to be somewhat erratic and of an extremely low magnitude making definition of the optimum modelling architecture difficult, therefore the best model was defined through comparison of predictions made using a number of models containing different quantities of hidden nodes on training and testing data. The optimum neural network model for prediction of ID weld metal acicular ferrite content was found to contain 8 nodes in the hidden layer. Predictions made across the training and test data domains with the optimum network architecture, shown in Figure 8.11, show a good correlation with the
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'y=x' ideal line. Outliers are seen to occur across the testing data with closely fitting predictions across the training data domain showing that the neural network has been trained well.

![Graph showing average sum squared error](image)

**Figure 8.10** – Average sum squared error for increased complexity of a neural network model for the prediction of ID weld acicular ferrite content

![Graph showing predicted vs actual AF%](image)

**Figure 8.11** – Predicted points, made using training and test data on a neural network model containing 8 hidden units, compared with measured values for the modelling of ID weld metal acicular ferrite content
Predictions across the training and test data domain, shown in Figure 8.11, are seen to be very good, considering the small data quantity used, although in order to evaluate the level of confidence in predictions it was necessary to investigate the $\sigma_w$ values. Perceived significance, $\sigma_w$, across input to output connections and input to hidden layer connections are shown in figure 8.12 (a) and 8.12 (b) respectively.

![Graph](image)

**Figure 8.12 (a)** – Perceived significance values, $\sigma_w$, across the input to output connections for a model of ID weld metal acicular ferrite content, containing 8 hidden units.
Figure 8.12 (b) – Perceived significance values, $\sigma_w$, across the input to hidden layer connections for a model of ID weld metal acicular ferrite content, containing 8 hidden units.

From the $\sigma_w$ values it is clear that the heat input from both ID and OD welding run plays a very strong role in influencing the ID weld metal acicular ferrite content, this was expected following inclusion of the OD heat input parameter to the modelling algorithm. Weld metal manganese (Mn), sulphur (S) and welder travel speed are also seen to carry a heavy influence on the modelling of ID weld metal acicular ferrite content.

8.3.2 Approach to modelling multiple ID weld metal microstructure constituents

A similar approach to that taken for the modelling of ID weld metal acicular ferrite was utilised to predict the entire weld metal microstructure using neural network techniques. The microstructure of the welds in question contained three main constituents, acicular ferrite (AF), primary ferrite (PF) and ferrite side-plate (FS). The same input structure was maintained as that in the modelling of acicular ferrite content in section 8.3.1, with the number of outputs increased from one to three. Once again the important parameters were considered to be the heat input at ID and OD, being representative of the re-heating that occurs during the OD welding process. The same quantity of data was available following pre-processing, and therefore the same 62 training and 62 testing data were utilised.
Values representing the error in training and testing of the neural network model for ID weld metal microstructure are seen in Figure 8.13. The optimum neural network model was found to contain 10 hidden units, although this was difficult to determine from training and testing error. Predictions for each individual output parameter are seen in Figure 8.14 (a) – (c), showing a good correlation between the ‘y=x’ ideal line and the predicted points across both training and test data domains. Prediction of FS and PF are seen to improve in comparison to the respective OD models, which can be explained by a better data distribution for ID weld metal microstructure as far as these output parameters are concerned.

![Figure 8.13 - Average sum squared error for increased complexity of neural network model for ID weld metal microstructure content.](image)

Perceived significance values, $\sigma_w$, across input to output layer connections and input to hidden layer connections are shown in Figure 8.15 (a) and (b) respectively. The $\sigma_w$ values placed on the heat inputs at the ID and OD are seen to lose the dominating influence as observed in modelling solely acicular ferrite content. A greater influence is placed upon the weld metal chemical content parameters which suggests that the rules formed around the data take into account more information as to the alloying and inclusion forming inputs. Weld metal Si, Ti and Mn are seen to carry greatest influence, with a varied response to other alloying inputs, with the three highest ranked chemical inputs all playing a vital role in formation of inclusions and refinement of the metal matrix.
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Figure 8.14 – Prediction of individual microstructural constituents, made using training and test data with a neural network model containing 10 hidden units, compared with measured data for ID weld metal (a) acicular ferrite content, (b) primary ferrite content, (c) ferrite side-plate content
Figure 8.15 (a) – Perceived significance values across input to output connections for neural network model for ID weld metal microstructure constituents, containing 10 hidden units

Figure 8.15 (b) – Perceived significance values across input to hidden layer connections for neural network model for ID weld metal microstructure constituents, containing 10 hidden units
8.3.3 Discussion of the modelling of weld metal microstructure

Detailed discussion of the modelling of weld metal acicular ferrite and microstructure has been presented in chapter 5 section 6, and the determining factors are similar to the work in this section. The formation of the microstructure in the OD welding relied heavily on both the thermal cycle applied and the chemical inputs responsible for the formation of inclusions and the promotion of a refined microstructure. Determination of the microstructure or quantity of a particular phase is further complicated at the ID weld bead due to re-heating taking place during the welding of the OD. The welding process at the OD produces a heat-affected zone (HAZ) causing tempering effects to a varying degree within the ID weld bead relative to the distance from the OD weld pool.

In modelling the acicular ferrite content of the ID weld metal it was found that the heat input at both ID and OD carried the greatest influence, along with a few key weld metal chemical characteristics. This showed a good correlation with what was expected from prior metallurgical knowledge, with the high concentration of acicular ferrite in the as deposited ID weld bead being altered upon re-heating during the OD welding process. This change is observed when considering the microstructure counts undertaken on both ID and OD weld metal, showing a much lower volume fraction of acicular ferrite in the ID weld metal. In the modelling of the overall weld metal microstructure more influence is placed up on the weld metal chemical characteristics, showing more distribution in the influence as expected considering the more complex nature of the outputs being mapped. A good correlation with measured results has been seen and when this work is combined with the models for OD weld metal a complete picture as to the weld microstructure of line-pipe can be ascertained.

8.4 Modelling of ID weld metal toughness

During the modelling of OD weld metal mechanical properties, it was found that the quantity of quality data was low and in order to increase this quantity for weld metal toughness the test temperature is also utilised. With the modelling of ID weld mechanical properties the quantity of data was found to be even less, and therefore modelling of ID weld metal toughness was the only mechanical property realistically achievable. The definition of the weld metal toughness taken at
the ID is as described for the OD, taken 2mm sub-surface from the ID of the pipe, as shown in Figure 8.16.

Figure 8.16 – Schematic diagram showing the relative position of the machined sample taken for ID weld metal toughness testing

8.4.1 Approach to modelling ID weld metal toughness

The modelling approach to weld metal toughness as described in chapter 7 section 3 was utilised in modelling the weld metal toughness for ID welds. The technique considered the weld metal chemistry and weld metal microstructure; parameters already shown to be predictable from welding process parameters in earlier work. The use of test temperature was once again key to the data structure allowing repetition of all other input data when mapped to the relevant weld metal toughness. The inputs used were; weld metal wt.% C, Mn, Si, Al, P, S, N, O and weld metal volume fraction acicular ferrite (AF) and primary ferrite (PF). The use of data regarding the weld metal microstructure removes the need for the complex number of inputs required to describe the heating and cooling processes that the weld metal undergoes, information which would require far more inputs for ID compared with OD.

Pre-processing of data undertaking normalising and randomising yielded 125 training data, 125 test data and 41 validation data. Input and output architecture were maintained, varying the number of nodes in the hidden layer to evaluate performance. Values of the error on the training and testing phases are shown in Figure 8.17, showing a good decrease in training error for
increased complexity, although the testing error is seen to increase with complexity and thus shows a degree of overfitting. Information gained from Figure 8.17 and a comparison of predictions made using models of increased complexity revealed the optimum neural network to contain 9 hidden units.

![Average sum squared error for increased complexity of a neural network model for ID weld metal toughness](image)

**Figure 8.17** — Average sum squared error for increased complexity of a neural network model for ID weld metal toughness

Predictions made across the training, test and validation data domains, using the 9 hidden units architecture are shown in Figure 8.18. Predictions across the training data domain are seen to fit the ‘y=x’ ideal line very closely, as expected from the results in Figure 8.17. Testing and validation data are seen to fit with the ‘y=x’ as a trend, with any outliers seen to carry large error bars indicating that the neural network is able to recognise the badly predicted points. Comparing the results for ID weld metal toughness, in chapter 7, a good correlation with measured values is seen, although in order to evaluate the robustness of the rules formed around the data the perceived significance values, $\sigma_w$, were again examined across the input to output connections, seen in Figure 8.19 (a), and across the input to hidden layer connections, shown in Figure 8.19 (b).
Test temperature is observed to carry the greatest influence across both input to output connections and input to hidden layer connections, explained by the greater influence over the data structure that this parameter holds. The small quantity of data used in modelling ID weld metal toughness, compared to OD weld metal toughness, relies on the use of test temperature far more to gain a useable dataset, and therefore it is expected that test temperature would carry such a dominant weighting. Of the other parameters, weighting is placed on acicular ferrite (AF), weld metal wt.% N, O, C, Al and P, all of which influence either inclusion characteristics, weld metal embrittlement or the performance of the weld under toughness testing.

Figure 8.18 – Predicted points of ID weld metal toughness, made using training, test and validation data, compared with measured data using a neural network architecture containing 9 hidden units.
Application of modelling techniques to the complete weld structure

Figure 8.19 (a) – Perceived significance values, $\sigma_w$, across input to output connections for neural network modelling of ID weld metal toughness, using 9 hidden units

Figure 8.19 (b) – Perceived significance values, $\sigma_w$, across input to hidden layer connections for neural network modelling of ID weld metal toughness, using 9 hidden units
8.4.2 Discussion of the modelling of ID weld metal toughness

Throughout the modelling of the ID weld metal characteristics a high level of influence has been found to be placed on OD welding process parameters. Weld geometry, microstructure and mechanical properties are all affected by the re-heating and pre-welding preparation that is a consequence of the OD welding process. Use of the weld metal microstructure as an input eliminates the need for the complex number of parameters relating to heating and cooling of the weld. The microstructure has been shown in the work in chapter 7 section 3, especially the acicular ferrite content, to carry a high influence on the weld metal toughness of OD weld metal. Throughout the literature modelling of weld metal toughness is seen to rely on microstructure characteristics\textsuperscript{64, 99}, although from the work in chapter 7 it is seen that a more complex combination of input parameters can be utilised.
8.5 Conclusions

- Successful modelling of the visible ID weld metal has been achieved, using neural network techniques. A model has been produced to predict measurable weld bead geometry, as a function of the ID welding process parameters and any information regarding the preparation of the parent plate with respect to the OD welding process.

- A model to determine the relative position of the ID weld bead compared to the OD weld has been developed, which successfully predicts the penetration depth of the OD weld, the distance between the measuring origin for ID and OD welds, and the points of contact between ID and OD weld edges.

- A combination of information predicted using the OD weld bead shape model, visible ID weld bead shape model and locator parameters have shown that the complete weld image for line-pipe can be derived solely from manufacturing process parameters. Prediction of the complete weld bead has been shown to carry a high level of accuracy for 3 wire welding, and lends itself to the combination with other modelling techniques.

- Modelling of weld metal microstructure and acicular ferrite content has been successfully undertaken, considering techniques developed for the modelling of OD weld metal. Development of the ID weld metal modelling has taken into account the re-heating effects of the OD welding process on the ID weld metal.

- A model for the ID weld metal toughness has been successfully created considering the characteristics of the weld metal at varying temperatures. Modelling inputs considered the use of microstructure and weld metal chemistry, although it has been shown in an earlier chapter that these are in turn predictable from process parameters.

- In this chapter it has been shown that the prediction, using neural network techniques, of ID weld metal characteristics are possible through consideration of the OD welding process in the modelling algorithm. Through combination with models for the OD weld metal the complete picture can be ascertained as to the full weld for single pass per side submerged arc welding of line pipe.
Chapter Summary

Neural network techniques previously applied to OD weld metal characteristics have been developed to accurately predict the more complex relationship between welding process parameters and the welding geometry, microstructure and toughness of ID weld metal. Due to the nature of the welding process undertaken in production of line pipe, the weld metal at the ID undergoes considerable changes during re-heating caused by the OD welding process. Throughout the work in this chapter it has been important to consider any attributable OD welding parameters that would have significant effect on the prediction of ID weld metal characteristics.

Modelling of visible ID weld geometry was shown to be highly dependent upon the preparation of the plate for both ID and OD. The plate preparation is directly related to the heat sink adjacent to the weld and thus influences the cooling and is related directly to final weld bead area\(^{15}\). Successful models have been developed in this chapter to ascertain both the visible ID weld geometry and the position of this geometry in relation to the OD weld, producing comparable results to those found in Chapter 6 for the OD weld bead shape\(^{127}\). A combination of the OD weld bead predictions, with the visible ID weld bead geometry, using the prediction of locator parameters, have shown excellent results as seen in Figure 8.9 (a) – (c). It is therefore possible to predict an entire weld bead shape accurately, which can be used as an input to other modelling approaches to form a complete ‘through process’ model.

The techniques previously developed for the prediction of OD weld metal toughness and microstructure have also been covered in this chapter, evolving the input architectures so as to recognise the effects of the OD welding process on the ID weld metal. The neural network models produced have been comparable, if not better, than those previously used in prediction of OD weld metal characteristics, which can be attributed to a far better spread of input and output data for the characteristics investigated. A combination of the models for ID weld metal characteristics with those developed in chapters 5, 6 and 7 for the OD weld metal allow for the prediction of important quality control parameters from process parameters for the complete weld. This will be a useful tool in both a manufacturing environment and theoretical modelling areas, giving a good insight into the trends present in welding without the need for costly, time consuming experimental trials.
Chapter 9 – Conclusions and Further Work

9.1 Introduction

Successful modelling of a range of characteristics of one pass-per-side multi-wire submerged arc welds from line-pipe has been developed throughout this thesis, considering weld metal chemistry, microstructure, mechanical properties and bead geometry. The conclusions in this section are presented in the same sequence of the chapters in the thesis.

9.2 Metallurgy of X100 line-pipe welds

The aim of the investigation of welds made using X100 line-pipe material was to characterise the inclusions and metal matrix resulting from the differing alloying additions found in the three series of welds described. Through optical microscopy techniques a definite increase in volume fraction of large lath size ferrite plates were seen through with weld series number, found to be relative to the levels of alloying elements present in the welds, in particular Ti and B. However, there were problems in the series 3 welds in distinguishing acicular ferrite laths from unaligned ferrite side-plate.

Investigation of the large ferrite laths and inclusions seen to be promoting their nucleation was undertaken using TEM analysis techniques, namely diffraction pattern and EDX analysis. No significant difference in the matrix structure was found between all of the weld series, with no significant variations in chemical composition and crystal structure; all measurements taken showing the crystal structure of the matrix to be BCC. With no significant findings with regards the ferrite matrix it was concluded that the changes in volume fraction of acicular ferrite and large ferrite laths was linked to the structure and chemistry of inclusions present.

FCC and BCC inclusions are present in the welds, with differing chemical composition. It was also observed that there is a distinct difference between inclusion centres and outer shells, showing that certain acicular ferrite promoting compounds are present on the inclusion surfaces. Ti rich inclusions are seen to be good nucleation sites for acicular ferrite microstructures, while Mn and Al rich inclusions are seen to be strong nucleation sites for the long ferrite laths. This is due to misfit between inclusion surface and ferrite matrix, a low misfit being required for
promotion of acicular ferrite growth. TiO$_x$ inclusions are seen to have low misfit values with the ferrite matrix. This is also seen for galaxite (MnAl$_2$O$_4$), although TiO$_x$ inclusion surfaces contain a higher number of particles thus creating a better chance of nucleation. High concentration Ti welds, such as the series 1 welds, are more likely to contain inclusions containing TiO$_2$, TiO$_3$ and TiO centres, with MnTi$_2$O$_4$ surface in series 2 welds where manganese content is relatively high, and a decrease in titanium is noticed. Series 2 and 3 welds having a lower Ti input will contain more alumina (Al$_2$O$_3$) and galaxite (MnAl$_2$O$_4$) inclusions, with the possibility of manganese sulphide forming depending on the level of sulphur impurity in the steels.

9.3 Neural network modelling of weld metal chemistry and microstructure

A neural network model for the prediction of weld metal composition has been developed, which produced accurate models using a 5 input architecture. It was interesting to note that the limits of scaling applied to the data were found to have a considerable influence over the achievable results, which were related to the limits of the activation function used. Normalising between the limits -0.5 and 0.5 was found to yield better results than using data normalised to give zero mean and standard deviation equal to 1. It is also apparent from this work that there is a lower limit to the amount of data that can be used in neural network modelling which is linked to the distribution of the data.

Simple neural network models considering plate and wire chemistry for a particular element are, in general, not significantly better than other existing methods such as multiple linear regression because there is an intrinsically simple physical relationship between weld, wire and plate chemical compositions. Improvements to the neural network modelling of weld metal chemistry have been identified through the use of a multiple output model. This approach gains an advantage over single output models because data regarding input chemistry for all modelled chemical elements is considered, thus taking into account the information required to consider the complex chemical reactions that take place in the weld pool.

A regression type model has been developed to predict the weld metal acicular ferrite content to a high level of confidence, taking into account important alloying elements and parameters influential to the weld thermal cycle. Multiple output models with the primary aim of predicting acicular ferrite, while also considering primary ferrite and ferrite side plate do not carry an
advantage over a singular output acicular ferrite model for the types of welds being considered. This is a result of the weld being in excess of 90% acicular ferrite content, and therefore the data distribution with respect to this output is far better in modelling terms than that of primary ferrite and ferrite side-plate. The techniques used in developing a neural network model for acicular ferrite have been successfully applied to both ID and OD weld metal. The more complex issues of re-heating that occur on the ID weld metal during the OD welding process are successfully accounted for through the use of additional heat input values from the OD welding.

A binary response model has been developed to predict the occurrence of hydrogen induced cracks in weld metal, using weld metal chemistry and basic welding parameters as inputs. This model is highly accurate within the range of the data domain for which it is trained. Training of binary response models requires a good balance between positive (1) and negative (0) response training patterns. It should be noted that a shift in this balance causes a shift in the responsive nature of the model, in the direction of the shift in balance of the data.

9.4 Neural network modelling of weld bead shape

It has been shown that neural network techniques can predict a weld bead shape to a high degree of confidence from manufacturing process parameters. The evidence suggests that the more measurements describing the weld bead shape profile, the better the accuracy of the predicted image. However, an efficient model can be made through the use of a smaller number of measurements for separate areas, with different neural networks being used to make predictions for such regions, providing that care is taken to ensure continuity at the overlapping points. Consideration of the relevance of each of the inputs to the output has also provided valuable insight into the effects of weld process parameters. The use of neural network models for the prediction of weld bead geometry has the potential for a detailed shape to be input into through-process models, rather than having to assume a shape from a limited number of defining parameters.

Attempts have been made to utilise neural network techniques to predict key geometry descriptors around the weld bead; namely weld width, penetration depth, cap height and measurements with respect to the flare region of the weld. The work has shown that these measurements have very little relation to the welding process parameters on their own, with the
Conclusions and Further Work

predictions made showing a high level of uncertainty. The way in which weld bead shape is described in respect of modelling from welding process parameters has been found to be a key issue in gaining good generalisation from the neural network models. The weld bead shape itself is a singular characteristic, although in order to define this in suitable terms for modelling it must be broken down into geometrical measurements defined throughout the chapter. It was found that penetration depth is classed as an independent shape characteristic, though all other geometrical parameters are dependent on the weld bead being classed as a whole or significant region of the weld. For example the weld width is determined by how much filler metal is deposited during the run of the lead wire and in some cases the second wire, thus is not independent and is related to the pre-determined penetration depth.

Successful modelling of the visible ID weld metal has been achieved utilising neural network techniques. A model has been produced to predict measurable geometry, utilising the ID welding process parameters and any information regarding the preparation of the parent plate with respect to the OD welding process. A model to determine the relative position of the ID weld bead compared to the OD weld has also been developed, successfully predicting the penetration depth of the OD weld, the distance between the measuring origin for ID and OD welds, and points of contact between ID and OD weld edges. The combination of information predicted using the OD weld bead shape model, the visible ID weld bead shape model and locator parameters have shown that the complete weld image for line-pipe can be derived solely from manufacturing process parameters. Prediction of the complete weld bead has been shown to carry a high level of accuracy for 3-wire welding, and lends itself to development of physical modelling techniques requiring knowledge of weld bead shape as an input.

9.5 Neural network modelling of weld metal mechanical properties

Successful neural network models have been developed for the modelling of weld metal toughness, weld metal true hardness and weld metal ultimate tensile strength (UTS) from weld process inputs for OD welds. Modelling of weld metal toughness has been successfully achieved using neural network techniques using weld metal chemistry and weld metal microstructure constituents for OD welds. It has also been possible to predict weld metal toughness using neural network techniques considering weld metal chemistry, simple welding process parameters and weld bead shape descriptors for OD welds. The use of such welding process parameters is seen
Conclusions and Further Work

throughout the literature to be related to the generation of good mechanical properties though the formation of an optimum weld microstructure.

The temperature at which the weld metal toughness is tested has been determined as a key parameter in this modelling, firstly due to the structuring of the weld data rows and secondly due to the intrinsic relationship between the temperature and the ductility of the steel. The acicular ferrite content was also observed as an important parameter in the modelling of weld metal toughness, independent of the data structure. However, acicular ferrite is not a readily available parameter from the manufacturing standpoint, and therefore modelling inputs must be included that represent this microstructural factor.

Comparable results to the modelling of weld metal toughness utilising weld metal chemistry and microstructure were achieved using the following input parameters; plate thickness, welder speed, measured heat input, weld metal wt.% C, Mn, Si Al, P, S, N, O, test temperature, cap height, weld width, bead penetration and flare region measurements. This indicates that through careful selection of the appropriate parameters representing all contributing factors attributable to the weld metal microstructure, the toughness of the weld can be accurately predicted using welding process variables alone. Predicted results of weld metal chemistry and weld metal acicular ferrite content have been successfully utilised in the neural network modelling of weld metal toughness. Utilising the same modelling architecture as that using measured variables a committee of neural networks were trained obtaining the desired inputs for weld metal toughness modelling from process parameters. Results of modelling with predicted inputs showed comparative accuracy with modelling using measured inputs, for the same input architecture.

Limited data resources for weld metal hardness and UTS meant that key parameters had to be omitted from the modelling architecture in order to obtain the maximum quantity of data. A neural network model has been successfully trained to predict weld metal true hardness utilising plate thickness, welder speed, weld metal wt.% Mo, Si, Al, Ti, P, S, N and O and a binary flag to identify the ID or OD run. The smaller quantity of data available for the modelling of weld metal hardness compared with weld metal toughness has shown that the rules formed around the data omit certain important metallurgical factors; heat input weld metal wt.% C and Mn. Similarly a successful model for the weld metal UTS has been developed, although this has been trained
using a very small quantity of data. The small quantity of data used in training therefore limits the domain of accuracy for this particular model.

Modelling of weld metal mechanical properties has been shown to be possible, using welding process parameters and information regarding welding consumables. The use of a committee of neural networks to obtain data not readily predicted from manufacturing information overcomes the problems related to key inputs not available at the production level. It is proposed that the principles here are easily applied to all weld metal characteristics provided sufficient data are available.

9.6 Further work

The driving force behind the work in this thesis comes from the need for a cost-effective tool to predict weld quality in the line-pipe manufacturing environment without the need for exhaustive testing and trials. The data considered in the neural network modelling of line-pipe welds in this thesis is for 3-wire experimental welds, using the same manufacturing route as a commercial operation would. Large diameter line-pipe welding is usually carried out using a combination of 4-wire welding at ID, and 5-wires for the OD welding process. It is proposed that the methods described in this thesis can be applied to weld metal chemistry, mechanical properties and geometry characteristics of 4 and 5-wire welds, with a minimum effort.

Work on the prediction of weld metal mechanical properties in this thesis was mainly concerned with toughness data; this was related to the quantity of information available. Through collection of more information with regards hardness, UTS or any other mechanical property of the weld metal more robust models can be developed. Utilisation of predicted or measured values of the microstructure content would further improve the results obtained; microstructure of the metal being vital to achieving good mechanical properties. Microstructure was not available to the modelling of weld metal hardness and UTS because of its limiting influence on the quantities of data available to the work.

The data used in modelling of weld metal hydrogen induced cracking (HIC), was small in quantity and it is proposed that given more examples of welds where HIC occurred a more robust model can be developed. The techniques can also be applied to the occurrence of sulphide stress.
Conclusions and Further Work

corrosion cracking in welded line-pipe resistance to which is key to good quality pipe for offshore sour service applications. Given sufficient data, regression type modelling can be applied to quantify the prediction of crack length occurring from HIC and SSCC phenomena.

Throughout this thesis it has been shown that the use of neural network data modelling is flexible and can be applied to a variety of quantifiable phenomena. It is proposed that the techniques in this chapter can be applied to other welding processes, using either single wire or multiple wire and single sided welding. The dynamic ability of the modelling technique surpasses the abilities of simpler regression modelling producing robust and accurate results for highly complex relationships not yet possible to model using physical principles.
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Results of energy dispersive x-ray (EDX) analysis on matrix of series 1 weld samples, results are for major constituents; other elements found were chromium and copper.

Appendix II

Section 1 – Training and test errors and predictions from the single output weld metal chemistry model; normalising to zero mean and standard deviation equal to 1, showing predictions from optimum 9 hidden unit models, and 1 hidden units linear models.

Section 2 – Results of training and test error from the single output model for weld metal chemistry; normalising between −0.5 and 0.5.

Section 3 - Predictions from the single output weld metal chemistry model; normalising between −0.5 and 0.5

Section 4 – Average weights across the multiple output neural network model, containing 8 hidden units, for weld metal chemistry

Section 5 – Weights on inputs for the neural network model, containing 10 hidden units, for weld metal acicular ferrite

Section 6 – Distribution of data for each element X used in the neural network modelling of weld metal acicular ferrite content. All data is normalised.
Appendix I
### Table of EDX Analysis Results

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Results of EDX analysis on matrix of series 1 weld samples. Results are for major constituents; other elements found were chromium and copper. EDX analysis undertaken on matrix samples has shown that the welds have a high concentration of ferrite, showing an average 96% Fe constituent.
Appendix II, Section 1
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Aluminium

Average Sum Squared Error

Number of Hidden Units

Aluminium - 5 Inputs - 9 Hidden Units

Aluminium - 5 Inputs - 1 Hidden Units

Predicted AI

Actual AI

Predicted AI

Actual AI
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Boron

Average Sum Squared Error

Number of Hidden Units

Boron - 5 Inputs - 9 Hidden Units

Boron - 5 Inputs - 1 Hidden Units

Predicted B

Actual B

Predicted B

Actual B
Appendices

Carbon

![Graph showing average sum squared error vs. number of hidden units.]

Carbon - 5 inputs - 9 hidden units

![Scatter plot showing predicted vs. actual C values.]

Carbon - 5 inputs - 1 hidden units

![Scatter plot showing predicted vs. actual C values.]

0.5
0.4
0.3
0.2
0.1
0.0

0
2
4
6
8
10

Number of Hidden Units

Average Sum Squared Error
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Copper

Average Sum Squared Error

Number of Hidden Units

Copper - 5 Inputs - 9 Hidden Units

Copper - 5 Inputs - 1 Hidden Units

Predicted Cu vs. Actual Cu
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Molybdenum

Average Sum Squared Error

Number of Hidden Units

Molybdenum - 5 Inputs - 9 Hidden Units

Molybdenum - 5 Inputs - 1 Hidden Units

Predicted Mo vs Actual Mo
Appendices

Nitrogen

Number of Hidden Units

Appendices Nitrogen 5 Inputs 9 Hidden Units

Appendices Nitrogen 5 Inputs 1 Hidden units
Appendix II, Section 2
Appendix II, Section 3
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Predictions made using optimum neural network architectures for weld metal chemistry prediction of element $X$, across the training data domain. (a) Weld wt.% C – 7 Hidden units, (b) Weld wt.% Mn – 5 Hidden units (c) Weld wt.% Si – 9 Hidden units, (d) Weld wt.% Al – 7 Hidden units, (e) Weld wt.% P – 7 Hidden units, (f) Weld wt.% S – 9 Hidden units, (g) Weld wt.% N – 7 Hidden units, (h) Weld wt.% O – 9 Hidden units
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Predictions made using optimum neural network architectures for weld metal chemistry prediction of element X, across the test data domain. (a) Weld wt.% C - 7 Hidden units, (b) Weld wt.% Mn - 5 Hidden units (c) Weld wt.% Si - 9 Hidden units, (d) Weld wt.% Al - 7 Hidden units, (e) Weld wt.% P - 7 Hidden units, (f) Weld wt.% S - 9 Hidden units, (g) Weld wt.% N - 7 Hidden units, (h) Weld wt.% O - 9 Hidden units
Appendix II, Section 4
Average weights across all inputs, considering input to output connections for a multiple output neural network model for weld metal chemistry, containing 8 nodes in the hidden layer.

Average weights across all inputs, considering input to hidden layer connections for a multiple output neural network model for weld metal chemistry, containing 8 nodes in the hidden layer.
Appendix II, Section 5
Weights on input to output connections for a 10 hidden unit neural network model for acicular ferrite

Average weights on input to hidden layer connections, for each individual input parameter, for a 10 hidden unit neural network model for acicular ferrite
Appendix II, Section 6
All data is plotted against plate thickness for a comparison

Welder Speed

Heat Input
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Wire Vertical Stickout

Wire Spacings
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Weld metal wt.% C (Carbon)

---

Weld metal wt.% Mn (Manganese)
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Weld metal wt.% Cr (Chromium)

![Graph showing the distribution of weld metal wt.% Cr.]

Weld metal wt.% Si (Silicon)

![Graph showing the distribution of weld metal wt.% Si.]

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Weld metal wt.% Ni (Nickel)

[Graph showing the distribution of normalized weight percent Ni against normalized plate thickness.]

Weld metal wt.% Al (Aluminium)

[Graph showing the distribution of normalized weight percent Al against normalized plate thickness.]
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Weld metal wt.% Ti (Titanium)

Weld metal wt.% P (Phosphor)
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Weld metal wt.% S (Sulphur)

Weld metal wt.% N (Nitrogen)
Appendices

Weld metal wt.% O (Oxygen)

Weld metal volume fraction acicular ferrite – AF%