INFLUENCE OF MATERIAL AND CONSTRAINT VARIATION ON THE FRACTURE TOUGHNESS BEHAVIOUR OF STEELS

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SCHOOL OF MATERIALS
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Along Crack Front ($B \leq 3 \text{ mm}, \text{Applied Loading} = 1000 \text{ N}$)

Satisfy That Condition.

(Note – R6 Equation III.7.4 is Relevant for Configurations Where $L \leq 0.5$ – Most of the MBL Analyses Here do not Satisfy That Condition.)

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ABSTRACT

The University of Manchester
Robert Stephen Kulka
Doctor of Engineering (EngD)
Influence of Material and Constraint Variation on the Fracture Toughness Behaviour of Steels
2012

The analysis of fracture toughness test data from standard specimens is often based upon the assumptions of planar crack fronts and homogenous material properties. However, these assumptions do not hold true for all test geometries or real components. The overall objective of this EngD was therefore to develop the methodologies used in fracture assessment of steel components, by incorporating a reduction in the conservatism inherent in the assessment procedures. These conservatism are associated with applying a ‘lower bound’ treatment to steel components, which in reality contain significant variability in effective fracture toughness, due to either material considerations (macroscopic or microstructural), or geometrical considerations including the effect of crack tip constraint.

The first method developed allows a comparison of a variation of fracture toughness values throughout a component, to a variation of the localised effective crack driving force. The main feature of this method takes advantage of the nature of the ductile-to-brittle transition regime of fracture toughness, where there is significant scatter. This leads to a probabilistic prediction of the location of fracture initiation, and a less conservative estimate of failure load, used to derive enhanced fracture toughness for the component. The second method calculates less conservative fracture toughness values for steels where there is significant heterogeneity in the dataset. The effects of measurement uncertainty on derived fracture toughness values can be monitored to improve probabilistic estimates of the heterogeneous fracture toughness values. These methods have been developed into predictive software tools, validated against data from the literature.

Finite element analysis of various configurations of compact tension and bend specimen, under different constraint conditions, was used to identify fracture mechanics parameters and constraint factors that will be of use in deriving accurate fracture toughness relationships from future testing programmes. The viability of low constraint specimens for accurately characterising increases in fracture toughness has been assessed. These recommendations enhance the relationships and advice suggested in the testing standards and literature. Loss of constraint in thin components can be quantified by a triaxiality parameter, which can be used to predict an increase in fracture toughness through use of a damage model, in this case developed based on a ductility exhaustion approach. This model can be used to predict initiation of ductile fracture in configurations with low constraint, leading to less conservative fracture toughness values, enhancing the guidance in the various defect tolerance assessment procedures.
DECLARATION

I, Robert Stephen Kulka, declare that no portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

Signed:...........................................................

Date:..............................................................
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# NOMENCLATURE

## ENGLISH SYMBOLS (LOWER CASE)

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>a</td>
<td>Half Crack Length</td>
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<tr>
<td>a_0</td>
<td>Initial Crack Size</td>
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<td>a_{eff}</td>
<td>Effective Crack Size</td>
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<td>n_L</td>
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**Knife Height, CTOD Test**
**ENGLISH SYMBOLS (UPPER CASE)**

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**Note:** The symbols represented here are mathematical notations used in fracture mechanics to describe various aspects of material behavior and response to loading conditions.
\( R_{\sigma} \) Function of \( T_B \)

\( S \) Distance

\( S_c \) Survival Function

\( S_{ij} \) Deviatoric Stress

\( S_{T0} \) Local Conditional Survival Probability

\( T \) Transverse Stress

\( T_i \) Temperature

\( T \) Traction Vector

\( T_0 \) Transition Temperature

\( T_{0(max)} \) Maximum Transition Temperature

\( T_{0deep} \) High Constraint \( T_0 \)

\( T_{0A} \) Transition Temperature for a Specific Constituent, \( A \)

\( T_B \) \( T_z \) Averaged Across Thickness

\( T_R \) Interim Transition Temperature

\( T_{ref} \) Reference Temperature

\( T_T \) Benchmark Transition Temperature

\( T_Z \) Out-of-Plane Constraint Factor

\( U_p \) Plastic Area Under a Load-Displacement Curve

\( V \) Volume

\( V_p \) Plastic Displacement at Crack Mouth

\( V_0 \) Reference Volume

\( W \) In-Plane Specimen Width

\( X \) Dimensionless Constant

\( Y \) Geometry (Compliance) Factor
<table>
<thead>
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<td>$\alpha$</td>
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<td>$\rho$</td>
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<td>$\sigma_{\text{YS}}$</td>
<td>Ultimate Tensile Stress</td>
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<td>Reference Stress (Yield Stress)</td>
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<td>Through-Thickness Stress</td>
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<td>$\sigma_f$</td>
<td>Principal Stress</td>
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<td>Incremental Displacement</td>
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<td>$\Phi$</td>
<td>Damage Parameter</td>
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<td>Angular Location on Crack Front</td>
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<tr>
<td>$\Gamma$</td>
<td>Contour for Line Integral</td>
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<tr>
<td>$\Pi$</td>
<td>Potential Energy</td>
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## ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>3PB</td>
<td>Three-Point Bend Specimen</td>
<td>HRR</td>
<td>Hutchinson, Rice and Rosengren</td>
</tr>
<tr>
<td>AGR</td>
<td>Advanced Gas-Cooled Reactor</td>
<td>LEFM</td>
<td>Linear Elastic Fracture Mechanics</td>
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<tr>
<td>AISI</td>
<td>American Iron and Steel Institute</td>
<td>LLD</td>
<td>Load Line Displacement</td>
</tr>
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<td>ASME</td>
<td>American Society of Mechanical Engineers</td>
<td>LSY</td>
<td>Large Scale Yielding</td>
</tr>
<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
<td>LT</td>
<td>Longitudinal-Transverse Orientation</td>
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<tr>
<td>BCC</td>
<td>Body Centred Cubic</td>
<td>LVDT</td>
<td>Linear Variable Differential Transformer</td>
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<td>BS</td>
<td>British Standard</td>
<td>MBL</td>
<td>Modified Boundary Layer</td>
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<tr>
<td>CCT</td>
<td>Centre Cracked Tension Specimen</td>
<td>MC</td>
<td>Master Curve</td>
</tr>
<tr>
<td>CEGB</td>
<td>Central Electricity Generating Board</td>
<td>M(T)</td>
<td>Middle Cracked Tension Specimen</td>
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<td>CMOD</td>
<td>Crack Mouth Opening Displacement</td>
<td>MML</td>
<td>Maximum Likelihood</td>
</tr>
<tr>
<td>CTOA</td>
<td>Crack Tip Opening Angle</td>
<td>PCPV</td>
<td>Pre-Stressed Concrete Pressure Vessel</td>
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<tr>
<td>CTOD</td>
<td>Crack Tip Opening Displacement</td>
<td>POR</td>
<td>Compact Tension Specimen with Additional Semi-Elliptical Surface Defect</td>
</tr>
<tr>
<td>C(T)</td>
<td>Compact Tension Specimen</td>
<td>PWR</td>
<td>Pressurised Water Reactor</td>
</tr>
<tr>
<td>DBT</td>
<td>Ductile-to-Brittle Transition</td>
<td>R-Curve</td>
<td>Resistance Curve</td>
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<td>EDF</td>
<td>Electricité de France</td>
<td>RKR</td>
<td>Ritchie, Knott and Rice</td>
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<td>EPFM</td>
<td>Elastic-Plastic Fracture Mechanics</td>
<td>SEN(4PB)</td>
<td>Single Edge Notched Four-Point Bend Specimen</td>
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<td>EPRI</td>
<td>Electric Power Research Institute</td>
<td>SEN(B)</td>
<td>Single Edge Notched Bend</td>
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<td>FAC</td>
<td>Failure Assessment Curve</td>
<td>SIF</td>
<td>Stress Intensity Factor</td>
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<td>Failure Assessment Diagram</td>
<td>SP</td>
<td>Single Point Estimate</td>
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<td>FCC</td>
<td>Face Centred Cubic</td>
<td>SSY</td>
<td>Small Scale Yielding</td>
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<tr>
<td>FE</td>
<td>Finite Element</td>
<td>TL</td>
<td>Transverse-Longitudinal Orientation</td>
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<tr>
<td>FEA</td>
<td>Finite Element Analysis</td>
<td>VBA</td>
<td>Visual Basic</td>
</tr>
<tr>
<td>HAZ</td>
<td>Heat Affected Zone</td>
<td>VCE</td>
<td>Virtual Crack Extension</td>
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1. INTRODUCTION

1.1 BACKGROUND TO THE PROJECT

As of August 2012, 30 countries worldwide are operating 435 nuclear reactors for electricity generation and 66 new nuclear plants are under construction in 14 countries. Nuclear power provided 13.5% of the world’s electricity production in 2010. In total, 13 countries relied on nuclear energy to supply at least one-quarter of their total electricity [1]. There are currently 16 operating nuclear reactors in the UK which normally generate about 18% of the UK’s electricity – 14 Advanced Gas-Cooled Reactors (AGRs), one Magnox reactor and one Pressurised Water Reactor (PWR). The last operating Magnox reactor – Wylfa 1 – is due to shut down when its fuel runs out, in September 2014 [2]. This will leave the seven twin-unit AGR stations and one PWR, all owned and operated by Électricité de France (EDF) subsidiary EDF Energy [3]. In 2009, EDF Energy took control of British Energy, who was the original owner and operator of these UK nuclear stations.

In AGRs, a controlled chain reaction generates heat which turns water into steam via boilers. At the heart of the reactor is a graphite core called the moderator, which slows down neutrons released by the uranium fuel so they will interact with other uranium atoms and sustain the chain reaction. Each reactor is encased in a pre-stressed concrete pressure vessel (PCPV).

In PWRs, heat from the reactor is transferred to the steam generators by circulating water under high pressure. The water cools the fuel, and also acts as a moderator for a sustainable reaction. The reactor, control rods and the pressurised water are contained in a steel reactor pressure vessel. This is connected to the steam generators, and a pressuriser, forming the sealed primary pressure circuit. The primary circuit is located within a PCPV.

The stations were designed to operate for long periods of time (30-40 years), but may be shut down now and then to allow for planned outages, as a response to safety concerns, or due to various trips or accidents. During these shutdowns, many of the critical components around the plant are inspected for any indications of defectiveness, including crack-like defects which may have appeared over time, for a variety of different reasons.

Defect tolerance arguments are made in nuclear safety cases for many components in nuclear facilities, as part of the argument for continued structural integrity. The arguments basically concede that many components in nuclear plant may be defective. This may be due to defects introduced during manufacture, or during operation. Defects that initiate during operation of nuclear facilities are actually fairly common, due to the intensive loading regimes that many
components undergo. Mechanisms that may contribute towards the initiation of defects include creep, fatigue and environmentally-assisted corrosion. However, it is important to note that the presence of a defect does not necessarily mean that the structural integrity of the component is compromised. All materials have an inherent resistance to fracture (the fracture toughness) and it is this material property which permits a certain level of defectiveness in a component.

Assessments of defect tolerance in UK nuclear facilities are carried out according to the R6 procedure [4], which is predominantly used by EDF Energy Nuclear Generation in the UK for demonstrating structural integrity of its fleet of nuclear power stations. However, R6 is also used in other civil nuclear programmes, as well as other industries, across the world to perform rigorous fracture assessment of components.

For obvious reasons, significant safety margins are imposed on assessments of defect tolerance in components. Stringent rules and requirements are placed upon nuclear operators to ensure that structural integrity of plant is one of the main areas of focus in the safety cases for continued operation. If the structural integrity of nuclear components is compromised, then there is a potential threat of radioactive release or a failure in the operation of the nuclear process.

Currently, all UK AGR stations are estimated to go offline by 2023 (Torness being the last, with Hinkley Point B and Hunterston B being decommissioned as early as 2016), with the UK’s only PWR (Sizewell B) due to be decommissioned in 2035. According to EDF Energy [5], the closure of old power stations, the decline of indigenous reserves of North Sea gas and the need to combat climate change means that the UK faces a potential ‘energy gap’. If new generating plants are not built soon then electricity supply could fall short of demand.

With nuclear incidents and accidents (most recently and notably, Fukushima) contributing to a recurring public fear regarding nuclear power, the political will for the construction of new nuclear power stations is another indeterminate aspect of the looming ‘energy gap’ crisis. Further efforts to provide life extension arguments for the current power stations have therefore never been more important and it is becoming extremely likely that EDF Energy will want to be able to make further arguments for many of its reactors. For a successful life extension argument, there are many assessments that need to be made, and these must include consideration of the time-dependent ageing mechanisms on the plant (such as neutron and hydrogen embrittlement, strain ageing, thermal ageing etc.), and time-dependent failure mechanisms (such as creep, fatigue and stress corrosion cracking).
1.2 PROBLEM DEFINITION

As many of the current nuclear facilities in the UK are reaching the end of their intended design life, there are significant political and commercial drivers to extend their operational life. To assist with enabling this life extension and to maintain the required safety standards, a re-examination of potential conservatisms within defect tolerance assessments is required. Additionally, with the production of new nuclear power generation facilities on the horizon, a refined appreciation of the behaviour of defects within high integrity components is advantageous. With a significant number of conservatisms removed, a cost efficient and safe design could be produced.

One of the key conservatisms inherent in standard defect tolerance assessments is the ‘lower bound’ treatment of the fracture toughness property, which is often mandated in deterministic assessments of steel components. However, in reality, steel components contain significant variability in effective fracture toughness, due to either material considerations (macroscopic or microstructural), or geometrical considerations, including the effect of crack tip constraint.

Constraint can be thought of as a measure of the hydrostatic stress triaxiality at a crack tip, with a reduction in triaxiality leading to an increased resistance to fracture.

Much work has been carried out over the last 40 years in developing single-parameter fracture mechanics, with rigorous testing methods available for deriving material fracture toughness properties, and there is wide understanding for how single-parameter theory may be used to undertake deterministic defect tolerance assessments. Two-parameter fracture mechanics is also fairly well understood, with methods available for estimating the loss of in-plane constraint in different configurations. However, there is some debate about the best way to incorporate two-parameter theory into fracture assessments.

The treatment of out-of-plane constraint loss in fracture assessments is not currently fully understood. Loss of out-of-plane constraint refers to the reduction of crack tip stress triaxiality, which occurs due to changes in geometry in the out-of-plane direction (generally the thickness of a component). There is currently no robust and accepted method to translate the effects of this phenomenon into a three-parameter fracture mechanics theory for use in assessments.

The effect of local material variation around a defect (microstructural and macroscopic) is also known to significantly affect local driving forces. Standard assessments are generally based on an assessment of the bounding material, or the ‘weakest link’ in a material combination, but a more refined appreciation of the effects of local material variation would be of great use in making a robust argument for the reduction of conservatisms.
1.3 GENERAL OBJECTIVES

The overall objective of this EngD is to develop the methodologies used in the fracture assessment of steel components, by incorporating a reduction in the conservatisms inherent in the assessment procedures. The work contained in this thesis investigates the conservatisms associated with applying a ‘lower bound’ treatment to steel components. The background to these conservatisms is highlighted in the literature review of Section 2, and the specific research aims for the thesis are then presented in Section 3. The purpose of the work is to allow improvements to be made to the R6 procedure, and other methodologies which share its principles, enabling more cost-effective design and accurate analysis of metallic components (potentially leading to plant life extension). The methods were developed primarily for use with components in the nuclear industry, due to its unique challenges surrounding the material degradation of metallic components in harsh environments and complex loading situations. However, the methods will be equally applicable in other industries.

The advances made during the EngD will increase the understanding of the fracture behaviour of steels under conditions of significant material and constraint variation. The results of the research have been used to produce benchmark methodologies and should be used to support future safety cases. In addition to the improved mechanistic understanding, tailored software tools have been developed to improve the modelling of material behaviour and provide simplistic advice for the reduction of conservatisms. The validated models and software tools will allow improved assessment methodologies to be developed, enabling more cost-effective design and analysis of metallic components.

Significant improvements may be made to defect tolerance assessment of thin section components, by making adjustments to the fracture toughness values used, accounting for the loss of constraint in both the in-plane and out-of-plane directions, relevant in various loading configurations. The viability of proposed low constraint specimens for accurately characterising increases in fracture toughness has also been assessed. Changes may also be made to provide less conservative fracture toughness values, based on an understanding of the variation of material properties around a crack front (including the effect of microstructural heterogeneity).

The improvements in understanding and the methods and tools developed should be used to suggest changes to the standard advice in R6 and other defect tolerance assessment procedures, for situations where the standard advice is significantly conservative. Recommendations are made in Section 8 as to the technical advances made during this thesis, which should be considered for inclusion in future revisions to defect tolerance procedures.
An additional objective is to provide the sponsoring organisation, Frazer-Nash Consultancy, with an enhanced fracture mechanics capability, and to help promote the company as a technical developer of defect tolerance assessment methodologies. Frazer-Nash Consultancy are at the cutting-edge of research and development in fracture mechanics, and the research contained in this thesis and carried out by the author during the course of the EngD will provide another platform for further developing this area of the business.

1.4 THESIS STRUCTURE

The structure of this thesis is as follows:

- A literature review providing technical background to the research projects and some of the common themes is presented in Section 2;
- The aims of the research are presented in Section 3;
- A discussion of the sponsoring organisation, and the motives behind the sponsorship of this EngD project are explored in Section 4;
- The first research project, looking at more accurate prediction of cleavage fracture using adjusted methodologies is presented in Section 5;
- The second research project, looking at the applicability of a thin width bend specimen for the characterisation of enhanced fracture toughness is presented in Section 6;
- The third research project, looking at the applicability of thin compact tension specimens for characterising out-of-plane constraint loss and the subsequent enhanced fracture toughness is presented in Section 7;
- A brief discussion regarding the knowledge gained from the research projects, and how this knowledge may be used to provide improvements to defect tolerance methodologies is presented in Section 8;
- General and specific conclusions from the EngD research project, and suggestions for further work are made in Section 9.
2. LITERATURE REVIEW

2.1 INTRODUCTION

The objective of this literature review is to summarise the current understanding in the area of the fracture mechanics assessment of defective metallic components. The basic concepts are introduced, with key areas more pertinent to the research being expanded upon. The concepts discussed are most relevant to (and often were developed for) the nuclear industry, but the approaches are transferable across any industry which demands integrity for its metallic components under highly demanding environments (e.g. the petrochemical and aerospace industries).

In particular, this review includes an appraisal of the current methods that are used to reduce some of the conservatisms inherent in the standard approaches for assessment of component fracture toughness. These conservatisms include the treatment of significant loss of constraint within a component (a reduction in crack tip stress triaxiality due to geometry and loading effects) and the treatment of significant heterogeneity in large datasets of fracture toughness. The gaps in the current knowledge and implementation of best practise are identified, and form the basis for the EngD.

This literature review is structured as follows:

- A brief discussion regarding the importance of refining best-practice fracture mechanics assessment for the nuclear industry is held in Section 2.2;

- Fundamental fracture mechanics concepts are discussed in Section 2.3;

- The effect of constraint on the fracture behaviour of steels is discussed in Section 2.4;

- Fracture mechanisms, and models that have been developed to understand and predict the micromechanical fracture behaviour of steels are discussed in Section 2.5;

- The Master Curve method, developed to describe the fracture toughness of steels in the transition region between ductile and brittle fracture regions is discussed in Section 2.6;

- Testing methods for determining fracture toughness values are presented in Section 2.7;

- The various fracture mechanics assessment methodologies are discussed in Section 2.8;
Concluding remarks on the findings of the literature review are presented in Section 2.9, summarising some of the gaps in the current knowledge, and consequently the areas upon which this EngD is focused.

2.2 NUCLEAR INDUSTRY

2.2.1 Defective Components

There are components in nuclear plant that, if their structural integrity were compromised, would threaten radioactive release or compromise operation of the nuclear process. Due to life extension programmes of ageing nuclear power stations, some of these components may be required to operate for a longer time than they were originally designed for. Safety cases that were produced to initially substantiate operation of plant components may no longer be appropriate, when these components have undergone significant degradation mechanisms (including some mechanisms which were not fully understood at the time of initial design and substantiation). Degradation due to prolonged exposure to high temperatures can reduce fracture toughness properties and initiate defects. The combination of these two effects can reduce safety margins.

There are two main ways that safety cases could be revised to improve tolerance to defects. The first way is to reduce the loads that plant components endure by reducing operating pressures and temperatures. However, this thesis assumes that station operators will resist the subsequent power output decrease (and consequent falls in revenue) associated with this. The second way is to make revisions to the current assessments that underpin the safety cases, through the reduction of assessment conservatisms. Subsequent plant inspections may then allow more favourable comparisons of any indications of defectiveness to these enhanced claims of defect tolerance. Conservatisms either inherent in the standard assessment procedures, or assumptions made about the loading configuration and associated material response will need to be challenged.

Paragraph 92(c) of the Safety Assessment Principles for Nuclear Facilities [6] states that a safety case needs to provide a demonstration that the nuclear facility will or does conform to good nuclear engineering practice and sound safety principles. It emphasises that a design should be based on deterministic engineering, defence in depth and adequate safety margins.

The safety case should identify the structures, systems and components that are important for the safe operation of the installation. The Technical Advisory Guide for the UK Nuclear Installations Inspectorate [7] states that the safety case should demonstrate that the integrity of structures, systems and components important for the safe operation of installation are maintained for a defined period of operation, taking due account of potential ageing and degradation mechanisms.
There are various components within nuclear plant that may require defect tolerance assessment, as can be seen in the schematics of nuclear power stations shown in Figure 1 and Figure 2 [8]. These may include pressurised vessels, pipes, reinforcing plates, supports, joints etc. The catastrophic failure of a reactor pressure vessel would almost certainly lead to unacceptable radiological consequences, and hence the highest standards are required to ensure the continuity of life for the pressure vessel. However, leakage from secondary pipework may be less significant particularly if detected prior to pipe break [6].

Pipework and pressure vessels include weldments, and the weld material used may sometimes have lower fracture toughness properties than the parent materials that the weldment joins together. Defects may initiate in these welded components during manufacture of the components, fabrication of the welds, or during service, as a result of creep, fatigue or environmentally assisted crack initiation under thermal or mechanical load cycling.

Figure 3 gives some examples of some of the types of defects that may be found in welds, based on some testing reported by Consonni et al. [9]. In order to assess these sometimes complicated geometries in a defect tolerance assessment, they are often simplified to representative crack-like defects, with elliptical or straight-edged geometries that circumscribe the area of interest. This makes it much easier to assess integrity, rather than assessing the response of the more complex defect geometries (especially those which have formed during fabrication e.g. due to a lack of fusion).

All nuclear plant that is assessed for structural integrity purposes is subject to a variety of loadings, which may include pressurisation, system loading (in large pipework systems long-range system loading can lead to significant bending stresses), local thermal stresses due to temperature differentials, and self-weight stresses. Welded components may also be subject to welding residual stresses and thermally-induced material mismatch (discontinuity) stresses.

During a structural integrity assessment it is necessary to demonstrate that all potential loadings during all normal operating and potential fault conditions are considered, with the most onerous loadings often posing the greatest threat to structural integrity. Pressurised thermal shocks are often analysed as a key loading for the PWRs, as significant stresses can be generated due to the severe system loading.

2.2.2 Materials

Common materials used in the construction of nuclear plant include ferritic and austenitic steels, nickel based alloys and associated weld materials. The two classes of materials of interest for the work reported in this thesis are ferritic and austenitic steels.
Austenitic stainless steels (or more accurately chrome-nickel steels, which are the grades where the austenite phase is stable at room temperature) [10], have a face-centred cubic (FCC) crystal structure and typically contain 18-30% Cr, and 8-20% Ni. Austenitic steels do not undergo a ductile to brittle transition, due to the increased mobility of dislocations in FCC crystals at low temperatures, allowing the material to remain ductile. They also have a high resistance to corrosion and have therefore they have become a very important group of steels for components that are required to undergo demanding environments. Austenitic steels generally undergo failure by fracture via a ductile mechanism, although some compositions have less resistance to a brittle fracture mechanism occurring.

Ferritic steels have lower alloy content than austenitic stainless steels [10]. They have a body-centred cubic (BCC) crystal structure. They are less corrosion resistant and less ductile than austenitic steels, however they have higher strengths and lower strain hardening. Ferritic steels can demonstrate a ductile fracture mechanism at elevated temperatures, but they undergo a transition in fracture mechanism from ductile to brittle fracture at lower temperatures, due to the reduced mobility of dislocations in BCC crystals at low temperatures.

Example microstructures of austenitic and ferritic steel [10] are shown in Figure 4.

The characteristics of welds are often very different to those of the parent material and depend substantially on the welding procedure used. The fracture behaviour of a weld material generally relates to the specific micromechanism of fracture. For ferritic welds this is a brittle or a ductile mechanism. These two mechanisms are discussed in greater detail later in the literature review.

2.3 FRACTURE MECHANICS FUNDAMENTALS

2.3.1 Background

The development of fracture mechanics as an engineering science has taken place over the latter part of the last century and much work has gone into improving the understanding of the fracture behaviour of different materials under different loading configurations. This section includes a brief summary of some of the basic theories, and specific research relevant to the research is highlighted in more detail. For a more in-depth history of the development of fracture mechanics over the years, books written by Anderson [11] and Milne et al. [12], and the review paper by Zhu and Joyce [13], amongst many others, provide excellent background discussion to the fundamentals of fracture mechanics.
2.3.2 Energy Release Rate

The first fracture-based relationships between the size of defects in components that fractured, and the stresses that caused them to fracture came from the work of Griffith [14]. The approach for quantifying fracture used an energy balance: for fracture to occur, the energy stored in a structure (from the work done by external loading) needs to be greater than the surface energy associated with the new surfaces created by the fracture process. Griffith originally developed this approach for brittle materials, based on evidence for the stress concentration effect discovered by Inglis [15].

In an ideally brittle solid, a crack can be formed by breaking atomic bonds. However, within metals, plastic deformation via dislocation motion can occur within the vicinity of a crack tip, resulting in additional energy dissipation. Irwin [16] and Orowan [17] independently made an adjustment to the Griffith method, to account for materials capable of plastic flow.

Irwin [18] later developed the energy approach to define the energy release rate, \( G \), as a critical crack driving force which is a measure of the energy required for crack extension. For a through-thickness crack, of length \( 2a \), in an infinitely wide plate, subjected to a remote tensile stress, \( \sigma \), \( G \) may be defined as:

\[
G = -\frac{d\Pi}{dA} = \frac{\pi\sigma^2 a}{E}
\]

where \( \Pi \) is the potential energy supplied by internal strain energy and external forces, \( dA \) is the incremental increase in the crack surface area following crack extension, and \( E \) is the Young’s modulus.

It is noted that \( G \) increases with crack size under stable crack growth, until it reaches a critical value of energy release rate, \( G_C \), when the crack will propagate (referred to as unstable crack growth). For materials and loaded configurations with a rising resistance curve (or R-curve), \( G_C \) is not a unique value. Examples of rising and flat R-curves are illustrated in Figure 5. Convention in the case of a rising R-curve is to define a \( G_C \) value for crack initiation (assuming a small amount of stable tearing prior to unstable crack growth), analogous to the 0.2% proof strength derived from tensile testing of materials that do not possess a distinct yield point.

The size and geometry of a component can have a significant influence upon the shape of the R-curve. A crack in a thin sheet tends to have a steeper R-curve when compared to the R-curve derived from a crack in a thick sheet. This is because a thin sheet is loaded predominantly in plane stress, while material near the tip of the crack in the thick plate may be in plane strain [11].
Figure 6 [19] shows a simplified comparison of the two states. In a thin body, stress cannot vary through the thickness significantly. Because a normal stress cannot exist on a free surface, the through-thickness stress, $\sigma_z$, must therefore be zero (i.e. plane stress). In a thicker body, the material is constrained in the thickness direction, and the through-thickness strain, $\varepsilon_z$, is close to zero (i.e. plane strain), and as a result a through-thickness stress must be developed.

In reality, conditions ahead of a crack tip are neither plane stress nor plane strain, but are three-dimensional. However, there are limiting cases where a two-dimensional approximation is valid [11]. In a real cracked structure e.g. a cracked plate subject to in-plane loading, the material near the crack front will be loaded to a higher stress than the surrounding material. Because of this, the material tries to contract in the other orthogonal directions, but is prevented from doing so by the surrounding material. Plane strain conditions therefore exist in the interior of the plate and the material on the plate surfaces is in a state of plane stress.

The measurement and subsequent interpretation of $G_C$ is therefore highly dependent upon the configuration of the loaded geometry.

2.3.3 Linear Elastic Fracture Mechanics

2.3.3.1 Stress Intensity Factor

Westergaard [20], Irwin [21], Sneddon [22] and Williams [23] were among the first to define closed-form expressions for the stress and displacement fields in the vicinity of a crack in a structure subject to external forces.

There are three generalised crack loading modes, as shown in Figure 7 [4]. For an infinite plate subjected to a remote tensile stress $\sigma$, with a through-thickness Mode-I crack with length $2a$, the leading term in the crack-tip stress field, $\sigma_{ij}$, for an isotropic linear elastic material, can be written as:

$$\sigma_{ij} = K_I \frac{f_{ij}(\theta)}{\sqrt{2\pi r}}$$

where $K_I$ is the Mode-I Stress Intensity Factor (SIF), $r$ is the distance from the crack tip and $f_{ij}(\theta)$ is a dimensionless function of the angle, $\theta$, at the position of the interest (see Figure 8 for definition of the coordinate axis). Williams’ solution provided the series expansion including this leading term, and also some higher-order terms. The SIF defines the amplitude of the crack tip singularity.

For a Mode-I loading configuration, Irwin [21] proved that $G$ and the Mode-I SIF, $K_I$, are uniquely related:
\[ G = \frac{K_I^2}{E'} \]

where \( E' = E \) for plane stress,

and \( E' = \frac{E}{1 - \nu^2} \) for plane strain.

where \( \nu \) is the Poisson's ratio. Irwin [21] also showed that when all three modes of loading are present, for any given geometry and loading configuration, the energy release rate is given by:

\[ G = \frac{K_{II}^2}{E'} + \frac{K_{III}^2}{E'} + \frac{K_{III}^2}{2\mu} \]

where \( \mu \) is the shear modulus, and \( K_{II} \) and \( K_{III} \) are the Mode-II and Mode-III SIFs, as illustrated in Figure 7.

Closed form expressions for the SIF, \( K \), have been derived for several geometrical and loading configurations, and many of the up-to-date expressions can be found in various texts, with common solutions found in stress intensity factor handbooks such as that of Rooke and Cartwright [24], Tada et al. [25], or the compendia of assessment procedures such as R6 [4] and ASME API579-1 [26]. For more complex situations, SIFs may be derived using linear-elastic finite element analysis (FEA).

All SIF solutions are of the form:

\[ K_I = Y\sigma\sqrt{\pi a} \]

where \( Y \) is a geometry and loading factor, often referred to as the compliance factor, and \( a \) is the crack length.

2.3.3.2 Plastic Zone Correction

The main problem with linear elastic fracture mechanics is that infinite stresses are predicted at the crack tip (as \( r \) tends towards zero, in Equation 2), but infinite stresses clearly do not exist in reality. Simple corrections were therefore derived to account for a moderate amount of yielding close to the crack tip. The two main approaches for dealing with this are the Irwin approach and the strip yield model.

The Irwin approach [27] assumes that a plastic zone ahead of the crack tip exists, with a size \( r_p \):
\[ r_p = \frac{1}{\pi} \left( \frac{K_I}{\sigma_{YS}} \right)^2 \] for plane stress, and

\[ r_p = \frac{1}{3\pi} \left( \frac{K_I}{\sigma_{YS}} \right)^2 \] for plane strain.

where \( \sigma_{YS} \) is the 0.2% yield stress. The plastic zone size is smaller under plane strain conditions because yielding is suppressed by the triaxial stress state (a higher constraint). The effective SIF, \( K_{eff} \), for a limited amount of plasticity can then be obtained by inserting \( a_{eff} \) (equal to \( a + r_p/2 \)) into the relevant SIF solution (Equation 7) for the geometry of interest.

Dugdale [28], Barenblatt [29], Burdekin and Stone [30] developed a strip yield model to account for limited yielding, which approximates the elastic-plastic behaviour by superimposing two elastic solutions: a crack under remote tension, and a crack with closure at the crack tip, as illustrated in Figure 9.

The strip yield model predicts:

\[ K_{eff} = \sigma_{YS} \sqrt{\frac{\pi a}{2}} \ln \left( \frac{\pi \sigma}{2 \sigma_{YS}} \right) \]

However, the plastic zone shape predicted by the strip yield model bears little resemblance to actual plastic zones observed in metals. The Irwin approach and strip yield model, compared in Figure 10, may extend linear elastic fracture mechanics (LEFM) beyond its normal validity limits, however they are only approximations. When non-linear behaviour becomes very significant, it should be taken into account in a more appropriate way.

### 2.3.3.3 Validity

If it is assumed that a material possesses a constant fracture toughness, \( K_C \), then there will be a critical combination of loading parameters contributing to \( K_I \) or \( K_{eff} \) (including \( a \), \( \sigma \), and \( \sigma_{YS} \)), at which a cracked material fails i.e. when \( K_{eff} \) is equal to \( K_C \). Under certain conditions, \( K_{eff} \) uniquely characterises the crack tip conditions when a plastic zone is present, and \( K_C \) remains a geometry independent material constant [11].

However, for this assumption to be appropriate, the plastic zone must be small to ensure plane strain conditions. In order for \( K_C \) to have any meaning, there must be a singularity dominated zone at the crack tip. When the plastic zone becomes too large, \( K \) no longer characterises the crack tip
stress state. According to ASTM E399 [31] and BS7448-1 [32], the following specimen size requirements must be met to obtain a valid measurement of $K_C$ in metals:

$$a, B, (W - a) \geq 2.5 \left( \frac{K_I}{\sigma_{YS}} \right)^2$$

where $a$, $B$, and $W$ are the crack length, thickness and in-plane width of the specimen respectively. As long as in-plane dimensions are sufficiently large to confine the plastic zone to the $K$-dominated zone, $K$ is a valid crack tip characterising parameter.

This does not necessarily mean that $K_C$ values obtained from fracture toughness tests that do not meet validity conditions are necessarily inappropriate for use in a fracture assessment, however the out-of-plane and in-plane loading conditions in the test should match those in the component of interest. This provision is often made use of in materials testing in the aerospace industry, when thin sheet testing of aluminium alloys is often required [11], and a more in-depth understanding of the micromechanics of the failure mechanisms is seen to be too costly.

### 2.3.4 Elastic-Plastic Fracture Mechanics

In many materials (and especially metals) it is not always sensible to characterise fracture behaviour using LEFM due to plasticity, and a more complex approach is often required. Two key parameters have therefore been developed to assist with the use of elastic-plastic (or non-linear) fracture mechanics (EPFM) techniques: the crack tip opening displacement (CTOD), and the $J$ integral. Each can be used as a fracture parameter in the case of larger amounts of crack tip plasticity when compared to LEFM – there are limits to their applicability, but these limits are less restrictive than the LEFM requirements described in Section 2.3.3.

#### 2.3.4.1 J Integral

Rice [33] applied the deformation theory of plasticity (i.e. nonlinear elasticity) to the analysis of a crack in a non-linear elastic material. He showed that the nonlinear energy release rate, $J$, could be written either in terms of the load-displacement response of a material, or as a path-independent line integral around a crack tip:

$$J = -\int_0^\Delta \left( \frac{\partial P}{\partial A} \right) d\Delta \quad \text{or} \quad J = -\int_\Gamma \left( wdy - T_i \frac{\partial u}{\partial x} ds \right)$$

where $\Delta$ is the incremental displacement, $P$ is the potential energy, $A$ is the crack face area, $w$ is the strain energy density, $x$ is the direction of crack growth, $y$ is the coordinate normal to the crack.
plane, $T_i$ are components of the traction vector, $u_i$ are the displacement vector components, and $ds$ is a length increment along the contour $\Gamma$, as illustrated in Figure 11.

Hutchinson [34], Rice and Rosengren [35] (HRR) showed that $J$ uniquely characterises crack tip stresses and strains in non-linear elastic materials. The $J$ integral is therefore both an energy parameter and a stress intensity parameter. They showed that crack tip stress fields, could be described by using an estimate of the material stress-strain response provided by the Ramberg-Osgood relationship [36]:

$$
\frac{\varepsilon}{\varepsilon_0} = \frac{\sigma}{\sigma_0} + a \left( \frac{\sigma}{\sigma_0} \right)^n
$$

where $\varepsilon_0$ is the reference strain, $\varepsilon$ is the strain, $\sigma_0$ is the reference stress (usually equal to the yield strength), $\sigma$ is the stress, $n$ is the strain hardening component and $a$ is a dimensionless constant (the yield offset).

The actual stress and strain distributions they derived are referred to as the HRR singularity:

$$
\sigma_y = \sigma_0 \left( \frac{J}{a\sigma_0^2 \varepsilon_0 I_n r} \right)^{\frac{1}{n+1}} \tilde{\sigma}_y(n, \theta)
$$

$$
\varepsilon_y = a\varepsilon_0 \left( \frac{J}{a\sigma_0^2 \varepsilon_0 I_n r} \right)^{\frac{n}{n+1}} \tilde{\varepsilon}_y(n, \theta)
$$

where $I_n$ is an integration constant that depends on $n$, and $\tilde{\sigma}_y$ and $\tilde{\varepsilon}_y$ are dimensionless functions of $n$ and $\theta$.

The $J$ integral therefore defines the amplitude of the crack-tip stress field for elastic-plastic hardening materials, just as $K$ characterises the linear elastic singularity (note the comparison of Equation 14 to Equation 2). A structure in small-scale yielding (SSY) therefore has two singularity dominated zones: one in the elastic region (i.e. where $n = 1$), where stress varies as a function of $r^{-1/2}$, and one in the plastic zone where stress varies as $r^{-1/(n+1)}$.

For the special case of a linear elastic material, $J$ is proportional to the square of $K$:
Clearly, the HRR singularity contains exactly the same problem as LEFM, in that as \( r \) tends to zero, infinite stresses are predicted. The HRR fields are not as accurate close to the crack tip, where the large strains reduce the stress triaxiality. For very small \( r \) values, the HRR solution is invalid because it neglects crack tip blunting. A blunted crack tip is effectively a free surface, and therefore the stress component in the plane of the crack reduces to zero at the crack tip.

However, the \( J \) integral is a useful fracture parameter, as long as there is a region close to the crack tip that can be described by the HRR criteria. When the HRR singularity is appropriate, the loading is proportional. However, when the higher-order terms in the solutions are significant, loading is often non-proportional and two-parameter solutions are required.

Landes and Begley [37, 38] were among the first to measure \( J \) experimentally, using multiple laboratory scale specimens with varying sized cracks, and determining the absorbed energy. Using Equation 12, the \( J \) integral could be derived. However, this method clearly has disadvantages in that multiple specimens must be tested and this is very costly.

Rice et al. [39] showed that it was possible, in certain cases, to determine \( J \) directly from the load-displacement curve of a single specimen (as illustrated in Figure 12):

\[
J = \frac{1}{B} \int_0^p \left( \frac{\partial P}{\partial a} \right) dP \quad \text{under load control}
\]

\[
J = -\frac{1}{B} \int_0^\Delta \left( \frac{\partial P}{\partial a} \right) d\Delta \quad \text{under displacement control, and}
\]

where \( P \) is the total load, and \( \Delta \) is the associated displacement.

A general relationship for estimating the \( J \) integral was then developed by Sumpter and Turner [40] for a variety of configurations can be written in the following form:

\[
J = \frac{K_r^2}{E} + \frac{U_p}{Bb} \eta_p
\]

where \( U_p \) is the plastic area under a load-displacement curve, and \( \eta_p \) is a dimensionless geometrical factor.
As a result of this work, the determination of the plastic eta factor $\eta_p$ simplifies the estimation of the $J$ integral from a single load-displacement curve. Paris et al. [41] pointed out that expressing $J$ in this way was only appropriate when the variables of geometry and deformation are separable (i.e. where the $J$ integral may be expressed as the product of two functions, one dependent on crack geometry, and the other on the material deformation behaviour), however Sharobeam and Landes [42] verified the separation relationship for ductile materials through detailed experimental work and finite element analysis. Further work was then performed to show that the $J$ integral could be used to characterise a material during the crack growth process, and the unloading compliance technique was developed by Clarke et al. [43] to permit construction of the $J$-$R$ curve for a growing crack using a single specimen.

In the 1970s and 1980s, the Electric Power Research Institute (EPRI) sponsored an estimation scheme for establishing a $J$ integral handbook [44], with $J$ integral solutions for many standard specimens under plane stress and plane strain conditions. However, most finite element analysis software nowadays has the capability to calculate the $J$ integral for more complicated loading configurations.

### 2.3.4.2 Crack Tip Opening Displacement

Wells [45] observed that in some test specimens of tough steels, crack faces had separated prior to fracture, due to extensive plastic deformation which had blunted the crack tip. He noticed that the amount of blunting was proportional to the apparent fracture toughness, and that therefore the crack tip opening displacement (CTOD, or $\delta$) could be used to characterise the fracture toughness of materials that did not exhibit LEFM behaviour. The CTOD was shown to be related to either the stress intensity factor, $K_i$, or the energy release rate, $G$, through the following expressions:

$$\delta = 2u_y = \frac{4}{\pi} \frac{K_i^2}{\sigma_{YS} E}$$

or

$$\delta = \frac{4}{\pi} \frac{G}{\sigma_{YS}}$$

where $u_y$ is the half displacement at the tip. The use of CTOD requires measurement of the $\delta$ value, associated with the onset of fracture, however such a measurement is subjective, and is the main drawback of the method. There are a number of alternative definitions of CTOD. The most common are: the displacement at the original crack tip; and the $90^\circ$ intercept (commonly used to infer the CTOD in a finite element analysis), which was originally suggested by Rice [33]. These definitions are illustrated in Figure 13.

The relationship between CTOD and the $J$ integral is:
\[ J = m \sigma_{ys} \delta \]

where \( m \) is a constant that depends on stress state and material properties (approximately 1.0 for plane stress conditions and 2.0 for plane strain conditions).

The relationship is valid for LEFM, but also can be applied to non-linear conditions. Shih [46] provided evidence for this, and demonstrated that the two quantities are equally valid crack tip parameters for elastic-plastic materials.

### 2.4 CONSTRAINT

#### 2.4.1 Validity of Single Parameter Fracture Mechanics

In certain configurations, the zone for which \( J \) is applicable (i.e. where the zone can be described by the HRR singularity) is vanishingly small, and a single parameter is not adequate for describing the material state in the vicinity of the crack. This is partly because of a compressive stress, transverse to the crack face (\( T \) stress) invalidating the assumptions allowing for the use of \( K \) and \( J \), but is also due to the influence of large scale yielding on the crack tip stress state. \( K \) becomes invalid when the plastic zone size is a significant fraction of the in-plane dimensions. The \( J \) integral becomes invalid as a crack tip characterising parameter when the large strain region reaches a finite size relative to in-plane dimensions, or when stable crack growth is significant compared to in-plane dimensions.

The thickness of a component has been known for some time to have a significant effect on its apparent fracture toughness, with a reduction in thickness leading to an increase in fracture toughness over the plane strain value. However, when the component becomes too thin, alternate mechanisms take place (either gross plastic collapse, or shear band localisation, causing apparent fracture toughness to sharply decrease).

To allow fracture mechanics methods to be used appropriately in structural integrity analysis, the fracture toughness values derived using tests need to be relevant to the structural application. This is why test standards generally enforce strict geometrical requirements. If the standard \( K \) and \( J \) terms become invalid, due to the crack-tip constraint loss caused by the configuration of the specimen or the size of the plastic zone, then additional understanding of the geometrical and material response is required.

Analyses by McClintock [47] showed that the single-parameter assumption is not valid for non-hardening materials under the fully plastic conditions, because the near tip stress and strain
fields depend on the loading configuration for the specific geometry. Crack depth and specimen size can therefore have a significant effect on the crack driving force, and subsequently the apparent fracture toughness. However, single parameter fracture mechanics may still remain approximately valid in the presence of significant plasticity, provided the specimen retains a relatively high level of triaxiality. Most laboratory specimens for measuring fracture toughness, such as the compact tension and three-point bend geometries, are designed to retain high levels of triaxiality at fracture.

Critical $J$ values, $J_C$, can be converted to equivalent $K_C$ values using Equation 16. However, this is strictly valid for structures that are elastically loaded, and if $J_C$ is independent of specimen size.

Equation 11 provides specimen size requirements to provide a valid measurement of $K_C$ in metals. As long as in-plane dimensions are sufficiently large to confine the plastic zone to the $K$-dominated zone, $K$ is a valid crack tip characterising parameter.

Size requirements for $J$-controlled cleavage can be expressed in the form of:

$$B, b_0 \geq \frac{M J_C}{\sigma_y} \quad \text{(ensuring sufficient constraint)}$$

$$\Delta a_{\text{max}} \leq X b_0 \quad \text{(limit on ductile tearing)}$$

where $M$ and $X$ are dimensionless constants, and $\Delta a$ is the crack extension. Anderson and Dodds [48] originally recommended $M = 200$, based on their fracture toughness scaling model and plane strain elastic-plastic finite element analysis (FEA). Subsequent work relaxed the advice on the definition of $M$, and the current test standard, ASTM E1820 [49] recommends a value of $M = 10$ and $X = 0.25$. However, these size limits only apply to cleavage without significant prior stable crack growth. In the upper transition region, cleavage is usually preceded by ductile tearing, so judgements usually need to be made regarding the validity of the $J$ measurements.

There has been significant effort in trying to extend fracture mechanics theory beyond the limits of the single parameter theory, to account for these problems, by introducing a second parameter to characterise the crack tip conditions, as discussed in the following sections.
2.4.2 In-Plane Constraint

2.4.2.1 T Stress

Linear elastic fracture mechanics theory normally neglects all but the singular term of the Williams [23] expression resulting in a single-parameter approximation of the near-tip fields. The first two terms of the expansion may be written as:

\[ \sigma_{ij} = \frac{K_i}{\sqrt{2\pi r}} f_{ij}(\theta) + T \delta_{ij} \delta_{ij} \]

where \( \delta_{ij} \) is the Kronecker delta. Larsson and Carlsson [50] illustrated the influence of the \( T \) stress (the first non-singular term) on the stress fields around the crack tip. Betegon and Hancock [51] later showed the \( T \) stress can have a significant effect on the shape of the plastic zone and the stresses within the zone.

When the \( T \) stress equals zero the first, singular term, uniquely defines the near-tip fields. Single parameter fracture mechanics theory is however only appropriate in this case, which is described as a high constraint condition. Negative \( T \) stress values cause a downward shift in the stress fields (and hence a loss of constraint). Positive \( T \) stresses cause an upward shift (and thus higher constraint), although the effect is less pronounced. These effects are illustrated in Figure 14.

In a cracked body subject to Mode-I loading, the \( T \) stress scales with applied load. The biaxiality ratio, \( B \), introduced by Leevers and Radon [52] relates \( T \) to \( K \):

\[ B = \frac{T \sqrt{\pi a}}{K_i} \]

This can be used to qualitatively describe crack tip constraint for various geometries. Kirk et al. [53], Hancock et al. [54], and Sumpter [55] all used the approach to estimate crack tip stresses for a given geometry. A compendium of \( T \) stress solutions for a variety of geometries was developed by Sherry et al. [56].

However, the \( T \) stress methodology has limitations, since it is an elastic parameter, and has limited relevance when significant plastic deformation occurs.

2.4.2.2 Q Parameter

Assuming small-strain theory, stress fields within the plastic zone ahead of the crack tip can be expressed as the sum of the HRR field and other terms. The higher order terms can be grouped together into a difference field, \( (\sigma_{ij})_{Dij} \).
\[ \sigma_{ij} = (\sigma_{ij})_{HRR} + (\sigma_{ij})_{\text{Diff}} \]

This difference field can also be expressed as the deviation of the stress field from that based upon a \( T \) stress of zero, \( (\sigma_{ij})_{T=0} \):

\[ \sigma_{ij} = (\sigma_{ij})_{T=0} + (\sigma_{ij})_{\text{Diff}} \]

O’Dowd and Shih [57, 58, 59] noticed that this difference field corresponds approximately to a uniform shift of the hydrostatic stress field in front of the crack tip, and hence defined the \( Q \) parameter as:

\[ Q = \frac{\sigma_{ij} - (\sigma_{ij})_{T=0}}{\sigma_0}, \text{ at } r = \frac{2J}{\sigma_0} \text{ and } \theta = 0 \text{ (in front of the crack tip)} \]

where \( Q \) defines the amplitude of the difference field (and is therefore a representative constraint parameter). O’Dowd [60] defined the \( Q \) parameter as a direct measure of the relative stress triaxiality ahead of the crack tip. The distance \( r \) from the crack tip was selected, to be far enough from the blunting region of the crack tip so as not to be influenced by the local effect of crack tip blunting but still within the fracture process zone.

Single parameter theory assumes that fracture toughness values obtained from laboratory specimens may be directly related to structural applications. This assumption is conservative since it is based on a fracture toughness derived from specimens with high constraint. Two-parameter theories, such as the \( J-Q \) theory, require that the constraint of the specimens match the structural constraint at fracture, i.e. the two geometries must have the same \( Q \) at failure, for the \( J_C \) value to be relevant.

The \( J-Q \) and \( J-T \) theories are equivalent under SSY conditions, however diverge under Large Scale Yielding (LSY) conditions. The \( Q \) parameter is more capable than the \( T \) stress parameter of describing the constraint effect for a variety of deformation levels.

### 2.4.2.3 The \( A_2 \) Parameter

A drawback of the \( J-Q \) theory is that it is based upon a numerical solution developed from FEA results. A rigorous theoretical analysis was therefore developed by Yang et al. [61], and they showed that the first three terms of the crack-tip stress field expansion could be defined as:
where the stress angular functions $\sigma_{ij}^{(k)}$ and stress exponents $s_k$ depend on the strain hardening exponent $n$, and $L$ is a characteristic length parameter that is often taken to be $L = 1$ mm. The parameters $A_1$ and $s_1$ are related to the HRR field by:

$$A_1 = \sigma_0 \left( \frac{J}{\alpha \sigma_0 \varepsilon_0 I_\alpha L} \right)^{-s_1} \quad \text{where} \quad s_1 = \frac{-1}{1 + n}$$

where the first term is effectively equivalent to the value of the HRR field at $r = 1$ mm, and the other two are higher-order terms, both having amplitudes described in terms of the constraint parameter $A_2$ (which may be determined through regression analysis or other curve fitting technique).

Chou and Zhu [62] found that $A_2$ is independent of the applied $J$ under LSY and is therefore a useful parameter to describe constraint during ductile tearing.

### 2.4.3 Out-of-Plane Constraint

In real structures, fracture toughness depends on both the in-plane and the out-of-plane stress field near the crack front. Kotousov [63] found that three-dimensional effects can significantly influence the stress distribution, and consequently the fracture behaviour of a component.

Amongst others, Neale [64], Kulkarni et al. [65, 66] and Shahani et al. [67] investigated the thickness (or out-of-plane effect) and found an increase in effective fracture toughness when the specimen thickness decreased. Figure 15 illustrates the effect of thickness on fracture resistance for aluminium Alloy 7075 T-6, based on tests performed on by Weitzman and Finnie [68]. It is clear from Figure 15 that there is a significant thickness effect on fracture resistance in this aluminium alloy, with the toughness increasing from a value of 25 MPa $\sqrt{m}$ under plane strain conditions (for a thickness greater than 3 mm) to a peak of 115 MPa $\sqrt{m}$ at a thickness of approximately 1 mm. A drop in fracture toughness is then observed at thicknesses below 1 mm (due to changes in the failure mechanism).

An out-of-plane constraint factor, $T_2$, was proposed by Guo [69, 70, 71], amongst others. This factor can be calculated simply from the in-plane ($\sigma_{11}, \sigma_{22}$) and out-of-plane stress components ($\sigma_{33}$), where subscripts may refer to Cartesian coordinates $(x, y, z)$ or polar coordinates $(\theta, z, r)$:
Kotousov and Wang [72] considered a similar form for $T_Z$, but with the denominator multiplied by Poisson’s ratio, $v$.

A $J-T_Z$ fracture criterion was then developed by Guo [71] to relate this factor to fracture of ferritic steels in the brittle-ductile transition region:

$$J_{ZC} = J_C F(R_s)$$

where $J_{ZC}$ is the fracture toughness accounting for the out-of-plane constraint loss, and:

$$F(R_s) = \frac{2}{3} (1 + v) + 3p(1 - 2v)R_s^{-2}$$

$$R_s = \frac{2}{3} \left( \frac{1 + T_B}{1 - 2T_B} \right)$$

$$T_B = \frac{1}{2h} \int_{-h}^{h} T_Z dz$$

where $p$ is a constant describing the material’s fracture sensitivity to stress triaxiality and is a value between zero and one (zero indicating a brittle fracture mode, and a value of one indicating a ductile fracture mode), $h$ is the thickness of the plate.

It is noted by She and Guo [73] that a full three-parameter theory e.g. $J-Q-T_Z$ or $K-T-T_Z$, has been difficult to achieve. Zhao et al. [74] were able to accurately describe the stress field around the crack front of semi-elliptical surface cracks using a $K-T-T_Z$ description, and this work was extended by Zhao [75] to describe the elastic-plastic stress field for an embedded elliptical crack in a plate. Meshii and Tanaka [76] indicate that it may be possible to correlate the increase in fracture toughness observed in fracture toughness testing, using a knowledge of the $T_Z$ parameter.

Figure 16 illustrates a comparison of the $T$ and $T_Z$ values found by Meshii and Tanaka [76], based on FE modelling.

Kim et al. [77] argued that as well as the triaxial stress state having an important effect on the out-of-plane constraint and the subsequent fracture ductility, that the Lode [78] parameter $\mu$ should also be used to describe the stress state:
where \( \sigma_1, \sigma_2, \sigma_3 \) are the principal stresses sorted from maximum to minimum.

Neimitz and Galkiewicz [79, 80] attempted to modify the strip yield model to account for the effects of an out-of-plane constraint factor as calculated by Guo [71], as well as in-plane constraint, and demonstrated that the failure assessment diagrams used within R6 etc. may benefit from a reduction in conservatism.

A three-parameter fracture mechanics theory does not appear to be fully developed at the current time. The theory would benefit from a robust fracture criterion, and the allowance for a prediction of an effective \( J_c \), based on an understanding of the in-plane and out-of-plane constraint.

### 2.5 FRACTURE MECHANISMS AND LOCAL APPROACH

#### 2.5.1 Overview

The three most common fracture mechanisms in metals and alloys are ductile fracture, cleavage (brittle) fracture, and intergranular fracture. The mechanisms of relevance to this research are ductile and cleavage fracture at low temperatures (i.e. no creep influence).

The cleavage fracture mechanism is characterised by unstable transgranular crack extension. A material that undergoes brittle fracture generally can be observed to have a well-defined crack initiation point. The brittle fracture process may initiate at a number of potential sites such as brittle second phase particles, exposed to an elevated stress and strain field, and the process absorbs very little energy with incremental crack growth (hence the fast fracture).

The ductile fracture mechanism is characterised by a stable crack extension due to formation, growth and coalescence of voids. This process results in slow, stable crack growth and generally absorbs more energy.

Austenitic steels generally undergo fracture via a ductile mechanism, although some compositions have less resistance to a brittle fracture mechanism. Ferritic steels can demonstrate a ductile fracture mechanism at elevated temperatures, but with a transition from ductile to brittle fracture, and subsequently lower fracture toughness properties, at lower temperatures. This transition curve is illustrated in Figure 17. The temperature at which this transition occurs is strongly dependent on
the material, the strain rate of the applied loading, and also on the level of constraint. Since the onset of brittle fracture depends on a ‘weakest link’ initiator, it results in variable initiation fracture toughness for multiple but similar specimens, and therefore statistical methods are required to define fracture toughness in the transition region.

Local approach methods to fracture have been developed, which are effectively mechanistically-based models of the fracture process (whether ductile or brittle), and identify fracture criteria based upon the ‘local’ stress or strains, rather than being dependent upon the global geometry of the component. Some of the more popular models are highlighted here.

2.5.2 Ductile Fracture

Ductile materials fail as the result of the nucleation, growth and coalescence of voids that initiate at inclusions and second phase particles under increasing levels of plasticity. The growth of the voids, by means of plastic strain and hydrostatic stress, form a macroscopic flaw, leading to fracture.

The ductile fracture toughness is usually defined around the onset of stable crack extension (at the transition from crack blunting to crack tearing), which may be characterised by a distinct change in the slope of the R-curve. This fracture toughness value is often referred to as the ductile fracture initiation fracture toughness, where the fracture toughness value is calculated at 0.2 mm of crack extension after crack tip blunting has occurred (analogous with the 0.2% proof stress measure in tensile tests).

During the loading of a crack, local strains and stresses become sufficient to nucleate voids. These grow as the crack blunts, linking with the main crack, and causing the crack to grow. Voids form around second phase particles, such as inclusions, when sufficient stress is applied to break the interfacial bonds between the particle and the matrix, or if the particle fractures. Argon et al. [81] developed a continuum model for fracture and discovered that void nucleation occurs more readily in a triaxial tensile stress field (high constraint). Dislocation models have also been developed to describe void nucleation. However, Van Stone et al. [82] found that experimental observations usually differ from both continuum and dislocation models, since void nucleation tends to occur more readily at large particles.

Many materials contain a bimodal (or trimodal) distribution of particle sizes. Bi-modal particle distributions can lead to local ‘shear’ fracture surfaces between large voids, since void nucleation and growth occurs preferentially in the larger particles, producing deformation bands at an angle to the loading direction, depending on the distribution of the particles. Ductile crack growth is stable under displacement-control because it produces a rising resistance curve. Under load-control,
ductile tearing can become unstable when the increase in crack driving force due to crack extension is more rapid than that of the J-R curve, as illustrated in Figure 18.

When a crack in a plate grows by ductile tearing, the crack generally exhibits a tunnelling effect, where it grows more rapidly in the centre of the plate due to the higher stress triaxiality in this region. This through-thickness variation of triaxiality produces shear lips, where crack growth near the free surface occurs at a 45° angle from the principal stress.

There are a number of mathematical models for void growth and coalescence. One of the most widely referenced models is that of Rice and Tracey [83]. The Rice and Tracey model gave the following approximation for growth rate, assuming an isolated single void:

\[
\frac{\dot{R}}{R} = 0.283 \dot{\varepsilon}_{eq} \left( \frac{1.5\sigma_m}{\sigma_{YS}} \right)
\]

where \(\dot{R}\) is the radius growth rate of the void, \(R\) is the radius of the void, \(\dot{\varepsilon}_{eq}\) is the equivalent plastic strain rate, \(\sigma_m\) is the mean stress, \(R_0\) is the void radius.

The Beremin [84] ductile fracture model is based upon the Rice and Tracey model of ductile void growth, modified to take account of work hardening, and assumes that failure occurs at some critical value of void growth:

\[
\ln \left( \frac{\bar{R}}{R_0} \right)_C = 0.283 \int_0^{\varepsilon_{eq}} \exp \left( \frac{1.5\sigma_m}{\sigma_{eq}} \right) d\varepsilon_{eq}
\]

where \(\bar{R}\) is the mean of the radial displacements of the void, \(\sigma_{eq}\) is the equivalent stress (von Mises stress), and \(R_0\) is the initial void radius.

Rakin [85] performed analysis of cylindrical and compact tension specimens of 22NiMoCr37 steel at 0°C, discovered that the critical value of \((\bar{R}/R_0)\) was equal to 2.73, and found that this value gave a reasonable prediction of the critical J integral at crack initiation. Wang and Shatil [86] performed similar analysis of EN8 structural steel (BS080M40), and found the critical value to be equal to 1.49.

Since the Beremin and Rice and Tracey models are based upon growth of independent voids, and do not take account of interactions between voids, nor do they predict ultimate failure, a separate criterion must be applied to characterise void coalescence. The Gurson model [87] describes a failure criterion, as a yield surface:
\[ \Phi = \frac{3}{2} \frac{S_y S_y}{\sigma_{ys}} + 2 q_1 f \cosh \left( \frac{3}{2} \frac{q_2 \sigma_m}{\sigma_{ys}} \right) - \left[ 1 + (q_1 f)^2 \right] = 0 \]

where \( S_y \) is the deviatoric stress, \( f \) is the void volume fraction, and \( q_1 \) and \( q_2 \) are two adjustable parameters found by Tvegaard [88] to be described fairly reasonably by 2 and 1 respectively. The \( \sigma_{ys} \) in this case is the yield stress after hardening has taken place, if any. However, the revised Gurson model was still incapable of predicting void interactions. Tvegaard and Needleman [89] later developed the model by introducing an additional function \( f^*(f) \) to account for void coalescence. The Gurson-Tvegaard-Needleman model is frequently used to characterise ductile damage, however it is often difficult to correlate with experimental data.

An alternative model for predicting void interaction by Rousselier [90] defines ductile damage evolution, by predicting the plastic potential, \( F \):

\[ F = \frac{\sigma_m}{\rho} - H + \sqrt{3} DB(\beta) \exp \left( \frac{C \sigma_m}{\rho \sigma_{ys}} \right) = 0 \]

where \( \rho \) is the density, \( B(\beta) \) is a term representing the material damage (calculated from the void volume fraction of the material), \( C \) and \( D \) are material constants, \( H \) represents the hardening of the material. Typical values for carbon-manganese steels [4] are \( C = 0.65 \) and \( D = 1.3 \).

Sherry et al. [91] reported a calibration of local approach models, for the NESC-1 spinning cylinder test, which was designed to address the assessment of ageing in reactor pressure vessels. The cylindrical specimen is shown schematically in Figure 19, and was manufactured from modified A508 Class 3 ferritic pressure vessel steel. The specimen contained a number of defects, with the most significant one being a surface-breaking through-clad defect of depth 75 mm. The cylinder was heated to a temperature of 290°C and rotated to simulate a pressure loading. The rotational speed was increased and at 2100 rpm, the inner surface of the specimen was sprayed with cold water at a temperature of 5°C, and the through-thickness temperature gradient was continuously monitored.

Parameters for the Rousselier model were obtained by calibration against test specimen data using two-dimensional large-strain elastic-plastic FEA to characterise stress, strain and damage in the critical regions. The Rousselier model parameters were obtained by tuning to data derived from notched-bar data with notch root radii of 10 mm, 4 mm and 2 mm, tested at 25°C and 150°C. The Rousselier constants derived were \( C = 0.98 \), 0.80 and 0.75 for parent, HAZ and clad respectively, with \( D = 2.0 \), 1.8 and 1.9 for parent, HAZ and clad respectively.
It should be noted that all of these ductile fracture models all have a weakness in that they only predict volumetric void growth and coalescence, and do not take account of shear fractures, as summarised by Thomason [92].

### 2.5.3 Cleavage Fracture

Cleavage fracture involves separation of material along specific crystallographic planes. The fracture path is transgranular. As discussed by Knott [93], cleavage fracture is often called brittle fracture, but it can be preceded by large scale plasticity and ductile crack growth.

The preferred cleavage planes are those with the lowest packing density, since fewer bonds must be broken and the spacing between planes is greater. In the case of BCC materials, like ferritic steels, cleavage occurs on \{100\} planes. At low temperatures, BCC materials fail by cleavage because there is a limited number of active slip systems, due to the increased amount of activation energy required for slip in BCC structures.

In order for cleavage to initiate, there must be a local discontinuity ahead of the crack sufficient to exceed the local bond strength. Cottrell [94] postulated that micro-cracks form at intersecting slip planes by means of dislocation interaction, however a more common mechanism involves fracture from inclusions and second phase particles that form micro-cracks within the plastic zone, as presented by Smith [95]. In mild steels, cleavage fracture often initiates at grain boundary carbides. In quenched and tempered alloys, the critical feature is often a spherical carbide or an inclusion. In some cases, where cleavage initiates, fast fracture does not occur, possibly due to crack arrest at a particle matrix interface or at a grain boundary (due to the differing stress and deformation states), causing crack blunting. Cracks must remain sharp for the stress on the atomic level to exceed the cohesive strength of the material and cause fast fracture.

Susceptibility to cleavage fracture is enhanced by almost any factor that increases the yield strength, such as low temperature, a highly triaxial stress state (high constraint), radiation damage, high strain rate, and strain ageing. The ductile-to-brittle transition part of the fracture toughness curve is effectively shifted to the right as a result of these effects.

The Ritchie, Knott and Rice (RKR) model [96] predicted that brittle fracture occurs when a critical fracture stress, \(\sigma_c\), is exceeded over a characteristic distance, \(r_f\), leading Anderson [11] to a prediction of the fracture toughness locus:

\[
\frac{J_c}{J_0} = \left[1 - Q\left(\frac{\sigma_0}{\sigma_f}\right)^{n+1}\right] \quad \text{at} \quad \theta = 0 \quad (\text{in front of the crack tip})
\]
where $J_0$ is the critical $J$ value for the $Q = 0$ small-scale yielding condition (i.e. high constraint). $J$-$Q$ loci can be plotted to show the relationship between $Q$ and $J$ for different geometry and loading configurations.

It is worth noting that the shape of the $J$-$Q$ locus depends on the failure mechanism. Equation 41 refers to stress-controlled brittle fracture, such as cleavage in metals, but strain-controlled fracture (ductile fracture) is actually less sensitive to crack tip constraint. Supposing fracture occurs when a damage parameter, $\Phi$, reaches a critical value ahead of the crack tip, then Anderson [11] suggests that the effect of the failure criterion on the $J$-$Q$ locus may be described as:

$$\Phi = \left( \frac{\sigma_m}{\sigma_0} \right)^\gamma \bar{\varepsilon}_{pl}^{1-\gamma} \quad (0 \leq \gamma \leq 1)$$

where $\sigma_m$ is the hydrostatic stress, $\gamma$ refers to strain-controlled fracture at $\gamma = 0$, and stress-controlled fracture at $\gamma = 1$, and $\bar{\varepsilon}_{pl}$ is the equivalent plastic strain.

Anderson et al. [97] found that for purely strain-controlled fracture, fracture toughness actually decreases with loss of constraint. This effect is illustrated in Figure 20. This occurs, because as $Q$ decreases, crack tip stresses decrease, but plastic strain fields (at a given $J$) increase, and therefore a smaller $J_c$ is therefore required for failure (accumulation of the required amount of plastic strain). Microvoid growth in metals is governed by a combination of plastic strain, and hydrostatic stress. Consequently, for $\gamma = 0.5$ (in the middle of stress and strain-controlled behaviour), $J_c$ values for initiation of ductile crack growth are generally insensitive to geometry (although tearing resistance increases with decreasing constraint). The relationship of Equation 41 is therefore clearly quite difficult to use in reality, partly due to the fact that constraint-based local approach methods are based upon continuum theory.

Various statistical models by Anderson, Stienstra, Dodds et al. [98, 99, 100] for describing fracture have also been developed to relate the crack tip stress fields to cleavage fracture toughness using a micromechanical failure criterion. The size and location of microstructural features that cause cleavage in metals, such as carbides or inclusions, influence the fracture toughness, and therefore cleavage fracture toughness can be subject to a considerable amount of scatter. The models treat cleavage fracture as a weakest link phenomenon, where the probability of failure is equal to the probability of sampling one of these fracture triggering particles. Anderson and Dodds [99] found that due to the scatter, the volume of the material sampled by the crack is important, since it alters the probability of finding a critical microstructural feature near the crack tip. Since the critical size
of particle depends on stress, which varies ahead of the crack tip, the failure probability, \( P_f \), must be integrated over a microstructural volume ahead of the crack tip:

\[
P_f = 1 - \exp \left[ -\int \rho dV \right]
\]

where \( \rho \) is the number of critical particles per unit volume, \( V \). This assumes that \( \rho \) depends only on the locally applied stress, e.g. a principal \( \sigma_1 \) stress or the hydrostatic stress, \( \sigma_m \).

The effective thickness of a body therefore must influence the cleavage driving force, since longer crack fronts sample more critical particles and therefore have a higher probability of cleavage fracture – this effect may be characterised by a Weibull \([101]\) distribution. The Beremin cleavage model \([102]\) allows the probability of cleavage fracture to be calculated based upon the principal stress field in a fracture process zone close to the crack tip. The probability of fracture, \( P_f \), is given by:

\[
P_f = 1 - \exp \left[ -\left( \frac{\sigma_u}{\sigma_u'} \right)^m \right]
\]

Where \( m \) is the Weibull modulus, specifying the amount of scatter in the statistical distribution, \( \sigma_u' \) is the scale parameter of the distribution, and \( \sigma_u \) is the scalar Weibull stress, defined as an integral over the plastic zone, \( p_z \):

\[
\sigma_u = \left( \frac{1}{V_0} \int_{p_z} \sigma_1^{m} dV \right)^{1/m}
\]

where \( V_0 \) is an arbitrary reference volume, usually taken to be 1 mm\(^3\) \([4]\). R6 [4] Section V.2.9.1 includes an example of the use of the Beremin cleavage model, based on fracture data obtained at -50°C for 25 mm thick bend specimens (BS4360 43A mild steel) with a range of \( a/W \) values. The \( J_C \) values obtained are plot in Figure 21 and the derivation of the Beremin parameters shown in Figure 22. For a \( V_0 \) value of 50 \( \mu \text{m}^3 \), values of \( m \) and \( \sigma_u' \) were found to be 19 and 1695 MPa respectively.

Sherry et al. \([91]\) reported a calibration of local approach models, for the NESC-1 spinning cylinder test, as described in Section 2.5.2 for the Rousselier ductile damage evolution model. Parameters for the Beremin model were obtained by calibration against test specimen data using two-dimensional large-strain elastic-plastic FEA to characterise stress, strain and damage in the
critical regions. The model was calibrated against high constraint fracture toughness data for parent material (using compact tension specimen data obtained at 0°C and 90°C) and HAZ material (using three-point bend specimen data at 20°C). The Beremin constants derived were $m = 49$ and $44$ for parent and HAZ respectively, with $\sigma'_{u} = 2296$ MPa and 2850 MPa for parent and HAZ respectively.

An alternative model by Wallin [103], assumed that, if the crack tip conditions are uniquely defined by $K$, it can be shown that critical values of $K$, $K_{IC}$, follow a characteristic distribution:

$$P_{f} = 1 - \exp \left[ -\left( \frac{K_{IC}}{K_{0}} \right)^{m} \right]$$

where $K_{0}$ is a material property dependent on microstructure and temperature (a normalisation factor) that corresponds to a 63.2% cumulative failure probability. If $K_{0}$ is known, the entire fracture toughness distribution can be defined. $m$ was found to be reasonably described for ferritic steels of interest by a value of 4.

The major problems with these weakest link models are that they predict zero as the minimum fracture toughness in the material (where $P_{f} = 1$), and that they generally overpredict the scatter found in real specimens. Törrönen et al. [104] found that by incorporating a conditional probability of propagation into the statistical model, using a three-parameter Weibull distribution [101], these limitations could be removed:

$$P_{f} = 1 - \exp \left[ -\left( \frac{K_{JC} - K_{min}}{K_{0} - K_{min}} \right)^{m} \right]$$

where $K_{min}$ is the theoretical lower bound of fracture toughness, and $K_{JC}$ is the fracture toughness of the material derived using $J$ integral values.

### 2.5.4 Ductile to Brittle Transition

In the ductile-to-brittle fracture toughness transition region, illustrated by Figure 17 for ferritic steels, cleavage fracture can be preceded by ductile tearing. On initial loading in the upper transition region, cleavage does not occur because there are no critical particles near the crack tip, however as the crack grows more material is sampled and cleavage may eventually occur after some stable crack growth.
It was shown by Rosenfield and Shetty [105] that the distance of cleavage initiation from the initial crack tip correlates well with an increase in fracture toughness, as illustrated in Figure 23, highlighting the potential for scatter in cleavage fracture toughness values. Hoagland et al. [106] found that in the upper transition region, cleavage propagation often displays isolated islands of ductile fracture – unbroken ligaments are often discovered behind the arrested crack tip.

Because of this effect, fracture toughness values in the transition region tend to be highly scattered. Wallin et al. [107, 108] developed a statistical model (called the Master Curve), based upon Equation 47, for fracture toughness data in the transition region. This model is described in the following section.

2.6 MASTER CURVE

2.6.1 Overview

The Master Curve (MC) method was shown by Wallin [108] to be applicable for practically all steels with a BCC structure. With the MC method, the fracture toughness in the ductile-to-brittle transition (DBT) region is described with a single parameter, the transition temperature, $T_0$ (in °C), at which the median fracture toughness, corresponding to a 25 mm thick fracture mechanics test specimen, is 100 MPa√m. An example Master Curve for A533B steel is shown in Figure 24. The basic form of the MC method is standardised in the ASTM standard E1921 [109].

2.6.2 The Basic Master Curve Model

The approach is based on a statistical brittle fracture model, described in Section 2.5.3, which allows for the variation of fracture toughness based on the following probability function:

$$P[K_{JC} \leq K_I] = 1 - \exp\left(-\frac{K_{JC} - K_{min}}{K_0 - K_{min}}\right)^{4}$$

where $P[K_{JC} \leq K_I]$ is the cumulative failure probability, $K_I$ is the Mode-I stress intensity factor (SIF), $K_{JC}$ is the fracture toughness, $K_0$ is a temperature and specimen size dependent normalisation fracture toughness that corresponds to a 63.2% cumulative failure probability, and $K_{min}$ is the theoretical lower bound of fracture toughness.

Wallin states [108] that on the lower shelf of brittle fracture ($K_{JC} \ll 50$ MPa√m for ferritic steels), Equation 1 may be inaccurate. This is because the initiation criterion, on which the model is based,
is no longer dominant. Instead, fracture is considered to be propagation controlled. \( K_{\text{min}} \) is therefore an imposed threshold (typically equal to 20 MPa\(\sqrt{\text{m}} \)) for limiting the inaccuracies in this region. This value was shown to be reasonable for ferritic steels but is only based on an empirical fit to the data, and may vary depending upon material and local conditions.

The MC describes the temperature dependence, \( T \), of median fracture toughness, \( K_{JC(\text{med})} \), through the following equations:

\[
K_{JC(\text{med})} = 30 + 70 \exp(0.019[T - T_0])
\]

\[
K_{JC(\text{med})} = K_{\text{min}} + (K_0 - K_{\text{min}}) \ln 2^{0.25}
\]

The MC model allows for a statistical size effect, of the form:

\[
K_{JC(s)} = K_{\text{min}} + \left( K_{JC(0)} - K_{\text{min}} \right) \left( \frac{B_0}{B_s} \right)^{0.25}
\]

where \( B_0 \) corresponds to the normalisation thickness (25 mm) and \( B_s \) to the specimen thickness (and in a regular specimen, the length of the crack front). MC expressions may also be derived for other failure probability bounds, where \( P \) refers to the probability bound of \( K_{JC} \) being less than calculated:

\[
K_{JC(P)} = 20 + \left( 11 + 77 \exp(0.019[T - T_0]) \right) \left( \frac{B_0}{B_s} \right)^{0.25} \cdot \left( \ln \frac{1}{1 - P} \right)^{0.25}
\]

It should be noted that the MC equations are considered to be empirical in nature, and even though fracture toughness values in ferritic steels generally appear to have similar temperature dependence, outlier behaviour cannot be completely ruled out.

Currently, \( T_0 \) values are derived, according to ASTM E1921, through static, elastic-plastic fracture mechanics tests performed on standard bend (SEN(B)) and compact tension (C(T)) specimens (as in Figure 25) with deep notches \( (a/W = 0.5) \). The \( J \)-integral values at cleavage fracture, \( J_C \), are derived through the analysis of load-displacement curves measured during the fracture toughness tests (see Section 2.7 for description of these tests).

The test temperature, \( T \), and the configuration of all the specimens should ideally be the same to simplify the data analysis, when calculating \( T_0 \). The test temperature should be selected to be as
close as possible to the expected $T_0$. The ASTM standard requires a minimum of six replicate tests which must meet certain criteria. $J$-integral values at fracture can be converted to appropriate fracture toughness values, $K_{JC}$, based on the following relationship under plane strain conditions:

$$K_{JC} = \sqrt{\frac{J_c E}{1 - \nu^2}}$$

For a set of derived $K_{JC}$ values, the difference between the test temperature and the transition temperature follows from inversion of the Master Curve equation, using the median value of $K_{JC}$:

$$T - T_0 = \frac{1}{0.019} \ln \left( \frac{K_{JC(\text{med})} - 30}{70} \right)$$

The specimen ligament $b_0$, must have sufficient size to maintain a condition of high constraint at fracture. The maximum capacity of a specimen is given by:

$$K_{JC(\text{max})} = \sqrt{\frac{E b_0 \sigma_{YS}}{30(1 - \nu^2)}}$$

Data that exceed this limit on derived $K_{JC}$ may be censored, according to the standard.

The example Master Curve plot of Figure 24 demonstrates the $T_0$ for tests of A533B steel at -75°C, which also had a $T_0$ of -75°C.

### 2.6.3 SINTAP Lower Tail Analysis

The SINTAP method [110, 111, 112] provides a description of the lower bound of fracture toughness in the transition region based on a number of small data sets. The method gives an estimate of the transition temperature (as described in the standard procedure) and then iteratively adjusts this estimate for undue influence of outlier values in the upper tail of the distribution. The method is not useful for separating out the individual constituents of a material with different $T_0$ values. It does not provide an estimate of fracture toughness for the tougher or weaker constituents of the material. Instead, it stops significantly high fracture toughness values unduly affecting the derived $T_0$ value. The lowest fracture toughness (highest $T_0$ value) is also monitored, to assess whether it is significantly different from the $T_0$ calculated for the entire dataset. This comparison has implications for understanding the level of heterogeneity in the dataset. Figure 26 provides a schematic of how the method works. Elements of the SINTAP method [111] are incorporated in the ASTM standard.
2.6.3.1 Stage 1 – Maximum Likelihood Estimation

The $T_0$ value for Stage 1 of the analysis is determined iteratively using Equation 56:

$$
\sum_{i=1}^{N} \delta_i \frac{\exp[0.019(T_i - T_0)]}{11 + 77 \exp[0.019(T_i - T_0)]} - \sum_{i=1}^{N} (K_{JC(i)} - K_{min})^4 \exp[0.019(T_i - T_0)] \left(1 + 77 \exp[0.019(T_i - T_0)]\right)^5 = 0 \quad 56
$$

where $N$ is the number of specimens tested, $T_i$ is the test temperature corresponding to $K_{JC(i)}$, $K_{JC(i)}$ is a valid $K_{JC}$ datum or a dummy value substitute for an invalid datum, $\delta_i$ is the censoring parameter (1 if the datum is valid, or 0 if the datum is a dummy substitute value). The $K_{JC}$ fracture toughness values should be size corrected, and also set to a value determined by Equation 55 if the censoring limit is violated.

2.6.3.2 Stage 2 – Lower Tail Estimation

The $T_0$ value for Stage 2 of the analysis is again calculated using an iterative process. Firstly, the $T_0$ found during Stage 1 is used as a benchmark value for the calculation of $K_T$ for each datum, as defined by Equation 57:

$$
K_T = 30 + 70 \exp(0.019[T_i - T_0]) \quad 57
$$

$K_T$ is then used as the new censoring limit for the data. Samples with fracture toughness values greater than this limit are given a new $\delta_i$ value $= 0$. A test value of $T_0$, $T_T$, can then be derived iteratively using Equation 56, with the revised values of $\delta_i$ for the population.

If this $T_T$ value is greater than the $T_0$ value from the previous iteration, then the Stage 2 process is repeated, using this $T_T$ as the new $T_0$ benchmark. The process repeats until $T_T$ is less than or equal to the $T_0$ value from the previous iteration, at which point the $T_0$ value is designated $T_K$.

If the number of specimens in the dataset $N > 9$, $T_K = T_K$ and the Master Curve and the failure probability bounds may be defined. However, if $N < 10$, the small set data correction from Stage 3 of the analysis is required. Even if $N > 10$, performing Stage 3 of the analysis provides an indication of the level of heterogeneity in the population.

2.6.3.3 Stage 3 – Minimum Value Estimation

The maximum value of $T_0$, $T_0(\text{max})$, is calculated using the non-censored data:
\[ T_{0(max)} = \max \left| T_i - \left( \frac{1}{0.019} \ln \left[ \frac{(K_i - K_{\min})}{\left( \frac{1}{\ln 2} \right)^{1/4}} \right] \right) \right| \] for \( \delta_i = 1 \) \[ T_K = T_K + \frac{14}{\sqrt{r}} \] where \( r \) is the number of brittle failures in the population. If the number of specimens in the dataset \( N < 10 \), a small data set correction is used to define \( T_K \):

If \( T_{0(max)} - 8^\circ \text{C} < T_K \), the data are considered likely to be homogeneous, and the \( T_K \) value may be considered to be representative of the dataset. Otherwise, there is an indication of heterogeneity, and \( T_{0(max)} \) should be taken to be the representative value. \( T_K \) is then set equal to \( T_{0(max)} \). For \( N < 10 \), a small data set correction is used to define \( T_K \):

\[ T_K = T_K + \frac{14}{\sqrt{r}} \]

for \( \delta_i = 1 \)

2.6.3.4 Master Curve Derivation

The Master Curve and the failure probability bounds may be defined using the values of \( T_0 \) derived at each stage (equal to \( T_0 \) from Stage 1, and \( T_K \) from Stages 2 and 3).

The uncertainty of the estimate may be derived using the estimate provided in Appendix X4 of the ASTM standard [109]:

\[ \sigma_{T_0} = \sqrt{\frac{\beta^2}{r} + \sigma_{\text{exp}}^2} \]

where \( \beta \) is the sample size uncertainty factor, defined in Appendix X4 of the ASTM standard [109], and \( \sigma_{\text{exp}} \) accounts for the contribution of experimental uncertainties, equal to 4°C, if standard calibration practices are used.

The ‘SINTAP Lower Tail’ analysis method is intended for macroscopically homogeneous materials. In reality, ferritic steels are not homogeneous and the fracture toughness properties may depend on the specimen location in the sample. These heterogeneities may be associated with welds,
heat affected zones (HAZ) or local carbide distributions. The MC approach has therefore been further developed to enable the analysis of heterogeneous data sets. Wallin et al. [113] developed algorithms applicable for both bimodal heterogeneities as well as random heterogeneities.

2.6.4 Bimodal Master Curve

The bimodal MC method developed by Wallin et al. [113] allows a dataset with two distinct populations (e.g. material constituents), to have $T_0$ values determined for each. The method is useful for situations such as the analysis of welded components, where the sampled material may include separate microstructural zones. The probability of sampling each population can be established along with the individual uncertainties.

When the population of a material consists of two combined distributions, the total cumulative probability of failure may be expressed as a bimodal distribution of the form:

$$P_f = 1 - p_A \exp \left( - \frac{K_{JC} - K_{min}}{K_{0A} - K_{min}} \right) - (1 - p_A) \exp \left( - \frac{K_{JC} - K_{min}}{K_{0B} - K_{min}} \right)$$

where $K_{0A}$ and $K_{0B}$ are the characteristic fracture toughness values of the two components (similar to the $K_0$ parameter of Equation 47), and $p_A$ is the probability of the fracture toughness belonging to the first distribution. These three parameters are derived through maximisation of the likelihood parameter, $L$, for a given dataset:

$$L = \prod_{i=1}^{n} f_{ci}^{\delta_i} \cdot S_{ci}^{1-\delta_i}$$

where $f_c$ is the distribution function and $S_c$ is the survival function:

$$f_c = 4p_A \left( \frac{K_{JC} - K_{min}}{K_{0A} - K_{min}} \right)^{\delta_i} \exp \left( - \frac{K_{JC} - K_{min}}{K_{0A} - K_{min}} \right) + ...$$

$$4(1 - p_A) \left( \frac{K_{JC} - K_{min}}{K_{0B} - K_{min}} \right)^{\delta_i} \exp \left( - \frac{K_{JC} - K_{min}}{K_{0B} - K_{min}} \right)$$

$$S_c = p_A \exp \left( - \frac{K_{JC} - K_{min}}{K_{0A} - K_{min}} \right) + (1 - p_A) \exp \left( - \frac{K_{JC} - K_{min}}{K_{0B} - K_{min}} \right)$$

The numerical iterative process is simplified by taking the logarithm of the likelihood:
\[
\ln L = \sum_{i=1}^{n} \delta_i \ln(f_{\delta_i}) + (1 - \delta_i) \ln(S_{\delta_i})
\]

The standard deviation of the \( T_0 \) values (\( \sigma_{T_0A} \) for the more brittle material component, and \( \sigma_{T_0B} \) for the more ductile component) and the occurrence probability may be derived with the following equations:

\[
\sigma_{T_0A} = \frac{22}{\sqrt{Np_A - 2}}
\]

\[
\sigma_{T_0B} = \frac{16}{\sqrt{r - Np_A - 2}}
\]

\[
\sigma_{p_A} = \frac{0.35}{\sqrt{Np_A - 2}}
\]

For a given bimodal population, the uncertainty for the bimodal outputs should be less than that calculated using the standard procedure.

An indication of heterogeneity may be determined by the satisfaction of the following expression:

\[
|T_{0A} - T_{0B}| > 2\sqrt{\sigma_{T_0A}^2 + \sigma_{T_0B}^2}
\]

Figure 28 provides an example of the Master Curve and bounds that may be derived using this method (from an analysis by Wallin [113] of A508 Cl.2 steel). It is noted that in this example, two distinct populations (with \( T_{0A} \) and \( T_{0B} \) values of +65°C and +12°C respectively) are obtained, compared to the standard analysis which would yield an estimate of 34°C.

### 2.6.5 Random Heterogeneity

The random heterogeneity method developed by Wallin et al. [113] can be used to describe a data population for a collection of several materials (such as a large database of welded specimens including parent, weld and heat affected zone materials), or for a distribution of heterogeneities within a material. In a randomly heterogeneous material, \( T_0 \) is assumed to follow a Gaussian distribution characterised by a mean \( T_0 \), and a standard deviation \( \sigma T_0 \). There are two main methods for estimating the distribution – the maximum likelihood (MML) method, which is the more sophisticated method, and the single point estimation (SP) method intended for quick engineering
assessment. The SP method gives a simpler estimate of the \( T_0 \) value than is derived through the MML estimation, but it is not as accurate. For small datasets, the MML method is preferable.

### 2.6.5.1 Single Point Estimation

All non-censored values are used to determine individual \( T_0 \) estimates:

\[
T_{0i} = T_i - \frac{1}{0.019} \ln \left[ \frac{(K_{JC} - 30)}{70} \right]
\]

The single point estimate is estimated using:

\[
T_{0SP} = \frac{\sum_{i=1}^{r} T_{0i}}{r} - 4
\]

The estimate includes a 4°C bias due to the non-symmetry of the MC distribution. Accounting for the average inherent scatter of the MC distribution (taken conservatively as 21°C), the standard deviation for the data set is taken as:

\[
\sigma_{T_{0SP}} = \sqrt{\frac{\sum_{i=1}^{r} T_{0i}^2 - \left( \frac{\sum_{i=1}^{r} T_{0i}}{r} \right)^2}{r}} - 441
\]

An approximate fracture toughness curve may then be derived from:

\[
K_{JC} = 20 + \left( 11 + 77 \exp \left[ 0.019 \left( T - T_0 - \frac{\sigma_{T_0}^2}{20^\circ C} \cdot (0.5 - P) \right) \right] \right) \cdot \left( \ln \frac{1}{1 - P} \right)^{0.25}
\]

for \( P \leq 0.5 \), and:

\[
K_{JC} = 20 + \left( 11 + 77 \exp \left[ 0.019 \left( T - T_0 - \left( \sigma_{T_0} + \frac{\sigma_{T_0}^2}{20^\circ C} \cdot (0.5 - P) \right) \right) \right] \right) \cdot \left( \ln \frac{1}{1 - P} \right)^{0.25}
\]

for \( P > 0.5 \).
2.6.5.2 Maximum Likelihood Estimation

The mean $T_0$ and $\sigma T_0$ value for the distribution is calculated, by maximising the likelihood of Equation 65. For a Gaussian distribution, the total survival probability for each data point is obtained by the integral:

$$S_c = \int_{-\infty}^{\infty} f_T \cdot S_{T_0} \cdot dT$$  \hspace{1cm} (75)

and the corresponding total distribution function for each data point is obtained by:

$$f_c = \int_{-\infty}^{\infty} f_T \cdot f_{T_0} \cdot dT$$  \hspace{1cm} (76)

where the probability density function for $T_0$ is:

$$f_T = \frac{1}{\sigma T_{0\text{MML}} \sqrt{2\pi}} \exp \left[ -\frac{(T_0 - T_{0\text{MML}})^2}{2\sigma T_{0\text{MML}}^2} \right]$$  \hspace{1cm} (77)

and the local conditional survival probability at $T_0$ is given by:

$$S_{T_0} = \exp \left[ -\left( \frac{K_{JC} - K_{\text{min}}}{K_0 - K_{\text{min}}} \right)^4 \right]$$  \hspace{1cm} (78)

where $K_0$ is dependent on $T$ and $T_0$, and the conditional density probability at $T_0$ is:

$$f_{T_0} = 4 \left( \frac{K_{JC} - K_{\text{min}}}{K_0 - K_{\text{min}}} \right)^3 \exp \left[ -\left( \frac{K_{JC} - K_{\text{min}}}{K_0 - K_{\text{min}}} \right)^4 \right]$$  \hspace{1cm} (79)

A simple criterion to judge the likelihood that the data represents a heterogeneous material is given by Wallin et al. [113]. If heterogeneity is likely, then the standard deviation from the MML estimate is greater than twice the uncertainty derived from the ‘SINTAP Lower Tail’ analysis:

$$\sigma T_{0\text{MML}} > 2\sigma T_{0\text{SINTAP}}$$  \hspace{1cm} (80)

An approximate fracture toughness curve may then be derived, by solving Equation 75 for fracture toughness, to yield a desired survival probability at a given temperature. Figure 29 provides an example of the Master Curve and bounds that may be derived using this method (based on
analysis by Wallin [113] of different weld data sets from the decommissioned Trawsfynydd reactor). It is noted that in this example, the MML estimate obtained is a mean \( T_0 = +47^\circ C \), with a standard deviation of 31\(^\circ\)C, in comparison to the standard analysis which would yield an estimate of \( T_0 = +59^\circ C \).

2.6.6 Constraint and the Master Curve

The MC transition temperature, \( T_0 \), has been related to the specimen constraint, expressed in terms of the elastic \( T \)-stress by Wallin [114]. The investigation suggested that a linear relationship exists between \( T_0 \) and the elastic \( T \)-stress:

\[
T_0 = T_{0\text{deep}} + \frac{T\text{-stress}}{10\text{MPa}/^\circ\text{C}} \quad \text{for } T\text{-stress} < 0 \text{ MPa}
\]

where \( T_{0\text{deep}} \) is the \( T_0 \) for a deeply cracked high-constraint geometry.

This relationship was based on analysis of fracture toughness behaviour measured using SEN(B) specimens with varying crack lengths. Studies by Wallin et al. [115] revealed more subtle differences between deeply cracked SEN(B) and C(T) specimens due to the different \( T \)-stresses generated by each geometry. It is noted that both geometries show positive \( T \)-stresses.

Equation 81 was shown to be conservative for C(T) specimens.

Equation 81 was based on the assumption that \( T \)-stress is negative. For positive \( T \)-stresses, a more appropriate relationship has been developed:

\[
T_0 = T_{0\text{deep}} + \frac{T\text{-stress}}{12\text{MPa}/^\circ\text{C}} \quad \text{for } T\text{-stress} < 300\text{MPa}
\]

Equations 81 and 82 appear to be contradictory. However, Wallin asserts [110] that one does not invalidate the other and that both are approximations.

A slightly better fit to the data would have produced a non-linear or bi-linear dependence to describe the constraint sensitivity. However, it would not produce radically different results. It should be noted that there are limitations associated with these relationships, in that they are based on linear-elastic analyses and are only based on SEN(B) behaviour. The applicability of the advice to different geometries has not been confirmed. There is currently no advice to suggest the effect of constraint on the Master Curve when it can no longer be described solely by \( T \)-stress.
2.6.7 Application of Master Curve Methodology to Realistic Defects

MC parameters are determined using test specimens with assumed ‘straight’ crack fronts and a uniform stress state along the crack front. This enables the use of a single $K_I$ value (or an effective $K_J$ value, derived from the applied $J$ integral) and a single constraint value (e.g. a value of $T$-stress) to describe the crack driving force for the whole specimen. For a real crack however, these assumptions are not necessarily valid. For example, a defect found by Cheverton et al. [116] during an evaluation of the effects of cladding on the propagation of flaws in light water reactor pressure vessels, had an unusual shape, which resembled a semi-elliptical surface flaw, with some small deviations (see Figure 30). Values of $K_I$ (or $K_J$), constraint and temperature vary along the crack front length, $s$, leading to local discrepancies in $K_0$ (the temperature and specimen size dependent normalisation fracture toughness that corresponds to a 63.2\% cumulative failure probability).

In order to safeguard against geometry effects, fracture toughness testing standards prescribe the use of highly constrained deep cracked bend specimens having a sufficient size to guarantee conservative fracture toughness values. However, it is not always possible to ensure high constraint. This led Wallin [117] to define the requirement for an adjustment to the cumulative failure probability, to account for an appropriate integral of the relevant parameters over the crack front:

$$P_f = 1 - \exp\left( \int_0^s \frac{K_{I\Phi} - K_{I\min}}{K_{I0\Phi} - K_{Imin}} ds \right)$$  \hspace{1cm} (83)

In order to identify the effect that this has on the fracture toughness estimate, the effective stress intensity factor, $K_{Ieff}$, may be derived, corresponding to a specific reference temperature (for example the minimum temperature along the crack front):

$$K_{Ieff_{ref}} = \left( \int_0^s \frac{K_{I\Phi} - K_{I_{min}}}{K_{I0\Phi} - K_{I_{min}}} ds \right)^{1/4} \cdot (K_{0_{ref}} - K_{I_{min}}) + K_{I_{min}}$$  \hspace{1cm} (84)

where $K_{I\Phi}$ is the local stress intensity factor, and may be obtained from stress analysis as a function of location (for example the angular location on the crack front, $\Phi$). $K_{0_{ref}}$ is the high constraint $K_0$ corresponding to a reference temperature, $T_{ref}$, along the crack front:
\[ K_{0Tref} = 31 + 77 \exp(0.019[T_{ref} - T_0]) \]

where \( K_{0\Phi} \) is the local \( K_0 \) value, based on local temperature and constraint, with the form:

\[ K_{0\Phi} = K_{iT, stress} = 31 + 77 \exp\left(0.019\left[T - T_{0, stress=0} - \frac{T \text{ stress}}{12MPa''C''} \right] \right) \]

The effective crack driving force, \( K_{effTref} \), therefore accounts for the local stress, temperature and constraint state along the crack front, as well as the crack front length. Wallin performed an analysis of the defect found by Cheverton et al. [116], described above, using both the standard and the enhanced Master Curve methods (treating the defect as having a semi-elliptical shape) and found that use of the enhanced MC method would yield some benefit over the standard method, but that the two methods gave similar answers for this case (see Figure 31).

### 2.7 FRACTURE TOUGHNESS TESTING

#### 2.7.1 Generic Testing Methods

Fracture toughness tests measure the resistance of a material to crack extension. Tests may provide a single value of fracture toughness or a resistance curve depending on the failure mode. There are several specimen configurations, some permitted by the standards, and others yet to be standardised. The accuracy of the measurement of fracture toughness clearly plays an important role in the application of fracture mechanics methods discussed so far to structural integrity assessment.

The vast majority of tests are performed on either compact tension (C(T)), single edge notched bend (SENB) specimens, and middle-cracked tension (M(T)) specimens. The basic geometry of these specimens is illustrated in Figure 25.

Since materials are generally not homogeneous, microstructure and mechanical properties are often sensitive to loading and crack growth direction. Sensitivity to orientation is particularly pronounced in fracture toughness measurement, since there may be particular planes of weakness in the material. BS 7448 [32] and ASTM E616 [118] state that orientation is extremely important to define carefully during testing.

In order to introduce cracks that are sufficiently sharp, to be applicable to general fracture mechanics, fatigue pre-cracking is usually carried out. However, this must be done in such a way as to not adversely influence the fracture toughness value. In order to ensure the validity of the
pre-crack, the crack tip radius at failure must be larger than the initial fatigue crack radius, and the plastic zone produced during fatigue cracking must be small compared to the plastic zone at fracture.

For simple tests of fracture toughness measurement, all that is required is measurement of applied load and the resulting displacement. Additional instrumentation is sometimes required to monitor crack growth. Measuring load is fairly simple, since most testing machines are equipped with a load cell. The most common way of measuring displacement is with a clip gauge [31]. A clip gauge must be attached to sharp knife edges located near the mouth of the crack, in order to ensure that the beams of the clip gauge are free to rotate. Other methods of measuring displacement include the use of a linear variable differential transformer (LVDT), or the potential drop technique. The unloading compliance technique from the ASTM standards E813 and E1152 [119, 120] allows crack growth to be inferred, since the specimen can be partially unloaded at any time in the test, to measure the elastic compliance of the specimen. This measurement can be related to the current crack length via a crack length-compliance relationship.

It is usually of interest to measure both the load-line displacement and the crack mouth opening displacement. Compact specimens can be designed so that these are identical, however in an SENB specimen they are not. The comparison bar technique described by Anderson et al. [121] may be used to infer the load line displacement in this case. In this technique, illustrated in Figure 32, a bar is attached to the specimen at two points aligned with the outer loading points. The outer coil of a LVDT is attached to the comparison bar, which remains fixed during deformation, while the central rod of the LVDT moves as the specimen deflects.

Side grooves are often machined into the sides of a fracture toughness specimen to maintain a straight crack front during pre-cracking and during the test. An analysis of the effect of side grooves by Andrews and Shih [122] showed that a specimen without side grooves can be subject to crack tunnelling and shear lip formation because of the low stress triaxiality (constraint) at the outer surfaces. Side grooving effectively removes these free surfaces, where the plane stress conditions exist. Typically, side-grooved specimens have a net thickness of 80% of the gross thickness. If the side grooves are any larger than this, lateral singularities may be produced, causing the crack to grow rapidly at the outer edges.

For materials that behave in a linear elastic manner, ASTM E399 [31] and BS 5447 [123] provide standard methods for determining $K_{IC}$. However, it is important to note that the $K_{IC}$ test often produces invalid results. Because of the strict size requirements, ASTM E399 [31] requires that validity checks are made on size, ensuring that failure occurs under plane strain and limited plasticity:
\[ B, a \geq 2.5 \left( \frac{K_{IC}}{\sigma_{YS}} \right)^2 \quad 0.45 \leq a / W \leq 0.55 \quad P_{MAX} \leq 1.1P_Q \]

where \( P_{MAX} \) is the maximum applied load and \( P_Q \) is the critical load. Validity checks must also be made on the fatigue pre-cracking that was carried out.

When a pre-cracked specimen is loaded to failure, load and displacement are monitored. The critical load, \( P_Q \), can be derived in various ways, depending on the load-displacement curve (as seen in Figure 33). Non-linearity in the load-displacement curve may be caused by plasticity or sub-critical crack growth. Crack length should be measured from the fracture surface, noting that the crack depth will likely vary through the thickness.

A provisional fracture toughness, \( K_Q \), may then be derived from:

\[ K_Q = \frac{P_Q}{B\sqrt{W}} f \left( \frac{a}{W} \right) \]

where \( f \left( \frac{a}{W} \right) \) is a known function for the given specimen geometry.

Because of the size requirements, it is often very difficult to measure a valid \( K_{IC} \). A material must either be very brittle, or the specimen must be very large. For steels, these tests are only possible to characterise fracture toughness for the lower shelf (cleavage); in the ductile-brittle transition region and the upper shelf, the \( J \) integral and CTOD are required to characterise fracture.

It should be noted that plane strain fracture toughness values are also sensitive to strain rate, and a decreased fracture toughness may be observed as the strain rate increases.

### 2.7.2 J Integral Estimation

ASTM standards E813 [119] and E1152 [120] both allow \( J \)-\( R \) curve testing. Both standards apply to C(T) and SENB specimens. The overlap between the two standards led to development of the most recent standard for measurement of \( J \), ASTM E1820 [49].

\( J \) can be determined from the load-displacement curve (as in Figure 12) in a standard fracture toughness test, in a similar manner to \( K \). \( J \) can be divided into elastic and plastic components, and derived using Equation 19. In order to generate a \( J \)-\( R \) curve, \( J \) is computed incrementally with updated values of crack length and ligament length. Test specimens should be side grooved in order to avoid tunnelling and to maintain a straight crack front. Critical \( J \) values, \( J_C \), can be
converted to equivalent $K_C$ values using Equation 16. However, this is strictly valid for structures that are elastically loaded, and if $J_C$ is independent of specimen size.

As discussed in Section 2.4.1, size requirements for $J$-controlled cleavage can be expressed in the form of:

$$B, b_0 \geq \frac{MJ}{\sigma_y} \quad \text{(ensuring sufficient constraint)}$$

$$\Delta a_{\text{max}} \leq Xb_0 \quad \text{(limit on ductile tearing)}$$

where $M$ and $X$ are dimensionless constants, and $\Delta a$ is the crack extension. Anderson and Dodds [48] originally recommended $M = 200$, based on their fracture toughness scaling model and plane strain elastic-plastic FEA. Subsequent work relaxed the advice on the definition of $M$, and the current test standard, ASTM E1820 [49] recommends a value of $M = 10$ and $X = 0.25$. However, these size limits only apply to cleavage without significant prior stable crack growth. In the upper transition region, cleavage is usually preceded by ductile tearing, so judgements usually need to be made regarding the validity of the $J$ measurements.

### 2.7.3 CTOD Testing

CTOD test standards BS5762 [124] and ASTM E1290 [125] are standardised methods for measuring fracture toughness in the ductile-brittle transition region. Figure 34 [126] illustrates the CTOD test. The methods typically assume a hinge model, as illustrated in Figure 13, where displacements are separated into elastic and plastic components:

$$\delta = \delta_{el} + \delta_{pl} = \frac{K_I^2}{m\sigma_y E} + \frac{r_p(W - a)V_p}{r_p(W - a) + a + z}$$

where $r_p$ is the plastic rotational factor (typically 0.44), $m$ is a constant (approximately 1.0 for plane stress conditions and 2.0 for plane strain conditions), $z$ is the knife height, and $V_p$ is the plastic displacement at the crack mouth, derived from a load-displacement curve. $r_p$ is not actually a constant value, but depends on geometrical and material effects, however 0.44 is typically a value used in absence of available information.
2.7.4 Testing Thin Specimens

As discussed previously, some materials exhibit a rising R-curve. Experimental analysis on a 7075-T6 aluminium alloy by Irwin et al. [127] found that $G_c$ decreased as thickness increased and reached a lower bound value denoted by $G_{IC}$ where plane strain deformation prevails. The appearance of the fracture surface also changed from a slant fracture in thin specimens to fully flat in thicker specimens. However, the nature of this transitional behaviour is very material-specific.

BS7448-4 [128] and ASTM E561 [129] outline procedures for determining R-curves, which do not contain a minimum thickness requirement, and therefore can be applied to thin sheets. However, they are only appropriate when the plastic zone is small compared to the in-plane dimensions.

One problem with testing thin sheets is that the specimens can be subject to out-of-plane buckling, leading to a mixed mode loading of the crack. Anti-buckling fixtures therefore need to be carefully fitted to the test rig, to allow specimens to slide freely, but prohibit out-of-plane movement, as illustrated in Figure 35 [130].

Since ASTM E561 does not contain requirements on specimen size or the maximum allowable crack extension, there is no guarantee that an R-curve produced according to the standard would be a geometry-independent curve. The in-plane dimensions must be large compared to the plastic zone for LEFM to be valid.

The crack tip opening angle (CTOA) was postulated as a method for characterising the fracture toughness of thin specimens. The CTOA is defined as the angle of the two crack surfaces 1 mm behind the crack tip. This method was developed to characterise the stable crack extension in thin structures under low constraint conditions. A standard test method for CTOA testing is provided in ASTM E2472 [131]. However, the use of CTOA as a failure criterion generally requires the use of FEA to determine the relationship between the critical CTOA and the geometrical constraint of the component, as highlighted by Newman and James [132], and so this makes the method complex and expensive.

Schwalbe et al. [133] recommended that a CTOD-$\delta_5$ parameter be used to test thin specimens, since it is able to correlate large crack extensions and can be suited to tests of thin-walled specimens. The CTOD-$\delta_5$ parameter offers the possibility for determining the fracture toughness and the crack driving force by measuring or calculating displacement of two gauge points located 5 mm apart on a straight line through the original pre-crack tip, illustrated in Figure 36. This method further reduces the conservatisms inherent in the characterisation of the crack driving force in thin sections through the $J$ integral or other similar methods. The $\delta_5$ parameter is also discussed in ASTM E2472 [131].
2.8 FRACTURE ASSESSMENT

2.8.1 Approaches

- Various procedures have been developed for analysing the potential for a structure to fail by fracture, but all follow similar principles. Some of these include:
  - R6 – Assessment of the Integrity of Structures Containing Defects [4];
  - ASME API579-1 – A Comprehensive Fitness-for-Service Guide [26];
  - RCC-M – Design and Construction Rules for Mechanical Components of PWR Nuclear Islands [134];
  - RSE-M – In-Service Inspection Rules for Mechanical Components of PWR Nuclear Islands [135];
  - ASME XI – Rules for Inservice Inspection of Nuclear Power Plant Components [136];
  - The Japan Society of Mechanical Engineers – Codes for Nuclear Power Generation Facilities - Rules on Fitness-for-Service for Nuclear Power Plants [137];
  - BS7910 – Guide on Methods for Assessing the Acceptability of Flaws in Metallic Structures [138];
  - FITNET – Fitness-for-Service Procedure [139];

Most of these procedures provide similar advice, with the main assessment methods generally based on the basic fracture mechanics understanding highlighted earlier in this literature review. Differences may exist however in some of the finer details of the assessments, such as the modification of an assessment to account for loss of constraint, or the treatment of the interaction between primary, secondary and residual stresses. Loading in a structure can be categorised as either primary or secondary stress. Primary stresses generally arise from externally applied loads and moments, while secondary stresses are localised and self-equilibrating through the cross-section.
R6 is the procedure of focus for this thesis, given that it is the main procedure used to support nuclear safety cases in the UK, however, the methods developed in this thesis would also be suited to other assessment procedures.

Simple analyses based on LEFM, that do not call on any of the complicated features of the above procedures, can be applied to structures where the crack tip plasticity is small compared to the size of the structure. Analysis of a linear elastic structure becomes relatively straightforward, once a $K$ solution is obtained. For a Mode-I loading, the SIF can be expressed in the form shown by Equation 7. An approximate margin against failure can then be obtained from the ratio of the SIF to the fracture toughness of the material.

However, structures made from materials with sufficient fracture toughness may not be susceptible to fracture, but may fail instead by plastic collapse. The limit load of a cracked structure can be determined in various ways, and various handbooks have been produced for common applications, such as that of Miller [141]. Finite element analyses may also be used to determine the limit load of complex geometries and loading, through load-deflection analyses.

In LEFM, primary and secondary stresses are treated identically. The distinction is only important in analyses that include the effects of plasticity. In these instances, the treatment of secondary stresses, especially residual stresses, is crucial in assessments. Much work has been done, for example by Ainsworth [142] and Hooton and Budden [143] to characterise their effects on structural integrity. Welding residual stresses can be complex to account for in fracture analyses, since detailed FEA may be required in order to understand their distribution, due to the large inhomogeneities that they introduce into the analysis.

Most fracture analyses are deterministic, in that the values used in assessment are single quantities. In practical situations however, it should be noted that there is usually some degree of uncertainty e.g. in crack size, loading and material properties. It is not usually possible therefore to predict the precise failure condition, and significant conservatisms are often included within assessments to allow for this. Detailed probabilistic fracture analyses can be used to quantify the probability of failure, for a set of parameters with definable variability.

### 2.8.2 Failure Assessment Diagram

Dowling and Townley [144] introduced the concept of a two-criteria failure assessment diagram (FAD) to describe the interaction between failure by fracture and collapse. The first FAD was derived from a modified version of the strip yield model. This approach was then developed by the Central Electricity Generation Board (CEGB), to become the main assessment procedure of R6 [4].
In the R6 approach, plasticity effects are taken into account through the formulation of a failure assessment diagram. A sample FAD is shown in Figure 37.

The simplest form of describing the FAD (Option 1) is with the following equation:

\[ f(L_r) = \left[ 1 + 0.5L_r^2 \right]^{3/2} \left[ 0.3 + 0.7 \exp\left( -0.6L_r^2 \right) \right] \]

where \( L_r \) is the measure of the proximity to collapse in the structure and can be described simply by:

\[ L_r = \frac{\sigma_{\text{ref}}}{\sigma_y} \]

where \( \sigma_{\text{ref}} \) is the reference stress, but can also be described by a ratio of an applied load (such as bending moment) to the limit load.

\( K_r \) is a ratio of the total SIF to the fracture toughness:

\[ K_r = \frac{K_p + K_s}{K_{\text{mat}}} + \rho \]

where \( K_p \) is the SIF due to primary stresses, \( K_s \) is the SIF due to secondary stresses, \( K_{\text{mat}} \) is the material fracture toughness, and \( \rho \) is a plasticity correction (and can take many forms and may be derived in different ways depending on the loading condition and particular assessment). Fracture is seen to be avoided if the assessed defect has a \( K_r \) and \( L_r \) combination within the failure assessment curve.

This simple method was developed over the years, and the current R6 approach is seen as a state of the art flaw assessment procedure. It contains three options for assessment, each with increasing complexity and requiring more information about the configuration of interest. Option 1 assessments (as above) are the simplest, using a lower bound failure assessment curve, for when relevant stress-strain data for the material is not available. Option 2 assessments are based on a reference stress model, developed by Ainsworth [145], and utilises the stress-strain curve for the material in question. Option 3 analyses are the most accurate, where the Option 3 failure assessment curve is inferred from an elastic-plastic analysis of \( J \) for the structure of interest, incorporating the stress-strain response of the material.

Attempts have been made to incorporate the effects of in-plane constraint loss into the R6 procedure, developed from the work of Neale [146], by modification to the failure assessment curve.
and the relevant fracture parameters. These adjustments have developed from work by Ainsworth and O’Dowd [147], Hancock et al. [54], Burstow and Howard [148] and Sherry et al. [149, 150]. R6 currently takes account of in-plane constraint in a particular specimen geometry, using a normalised parameter, defined in terms of the constraint parameters, $T$ and $Q$, using the following relationships:

$$\beta_T = \frac{T}{L_r \sigma_y} \quad \text{or} \quad \beta_Q = \frac{Q}{L_r} \quad \text{where} \quad L_r = \frac{\sigma_{ref}}{\sigma_y}$$

R6 contains a compendium of $\beta$ solutions for various geometries, although only $\beta_T$ solutions are currently included. For values of $\beta_T$ greater than zero (signifying high constraint), there is no benefit to the inclusion of constraint effects in the assessment of defect tolerance, and the standard procedure of R6 is therefore used. $\beta_T$ values may then subsequently be used in R6 to provide a correction to the standard assessment methods, through modification of the FAD or the fracture toughness used. Figure 38 shows the types of adjustments that are made to the Option 1 Curve to account for various levels of in-plane constraint loss.

There are currently no specific recommendations in R6 for how the beneficial effects of out-of-plane constraint loss may be taken into account.

### 2.9 CONCLUSIONS FROM THE LITERATURE REVIEW

The following conclusions can be drawn from the literature review:

- As nuclear power stations reach the end of their lives, there is a desire to refine fracture mechanics assessments to reduce some of the inherent conservatisms in the assessment of the structural integrity of the plant. Reduction in these conservatisms may enable the safe extension of the lifetime of existing plant and also allow more efficient designs of components to be created in the future.

- A significant amount of work has been done developing single-parameter fracture mechanics over the decades, rigorous testing methods are available for developing fracture criteria, and there is wide understanding for how single-parameter theory may be used to undertake deterministic fracture assessments.

- Two-parameter fracture mechanics is also fairly well understood, with methods available for estimating the loss of in-plane constraint in different configurations. However, there is some debate about the best way to incorporate two-parameter theory into fracture assessments, with
the most benefit only claimed when constraint correction and local approach models are used in harmony with significant materials testing data.

- The treatment of out-of-plane constraint loss in fracture assessments is not currently fully understood. Recent studies of the loss of out-of-plane constraint have highlighted that a manipulation of the triaxial stress state could be used to define an out-of-plane constraint parameter, which in turn could be used to describe an increase in apparent fracture toughness. However, the translation of this parameter into a fracture criterion for use in a robust three-parameter fracture mechanics theory currently appears elusive.

- A robust method does not appear to exist to account for significant constraint effects on the apparent fracture toughness in the ductile-to-brittle transition curve, including the treatment of localised constraint effects found in geometries with complex defect shapes.

- Heterogeneity (non-homogeneity) in fracture toughness datasets in the ductile to brittle transition regime, where there is often significant scatter due to a bimodal or a random distribution of particles, cannot be accounted for adequately using the Master Curve methods provided in the standards.
2.10 FIGURES

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3. RESEARCH AIMS

3.1 OVERVIEW

The overall objective of this EngD is to develop the methodologies used in the fracture assessment of steel components, by incorporating a reduction in the conservatisms inherent in the assessment procedures. The work contained in this thesis investigates the conservatisms associated with applying a 'lower bound’ treatment to steel components, which in reality contain significant variability in effective fracture toughness, due to either material considerations (macroscopic or microstructural), or geometrical considerations including the effect of crack tip constraint.

The purpose of the work is to allow improvements to be made to the R6 procedure, and other methodologies which share its principles, enabling more cost-effective design and accurate analysis of metallic components (potentially leading to plant life extension). The methods have been developed primarily for use with components in the nuclear industry, due to its unique challenges surrounding the material degradation of metallic components in harsh environments and complex loading situations. However, the methods will be equally applicable in other industries.

3.2 THE EFFECT OF MATERIAL AND CONSTRAINT VARIATION ON CLEAVAGE FRACTURE TOUGHNESS

The analysis of fracture toughness test data from standard specimens is often based upon the assumptions of planar crack fronts and homogenous material properties, since this allows for the simplified manipulation of data. However, these assumptions do not hold true for all test geometries or real components.

A robust method does not appear to exist to account for the effects of significant levels of constraint loss on the apparent fracture toughness values relevant to the ductile-to-brittle transition regime.

The objectives of this phase of work are therefore to:

- Develop a prediction tool, validated against data from the literature, which will allow a user to identify the probable failure load and the likely location of fracture initiation in a given defective
component, based on an understanding of the nature of the ductile-to-brittle regime of fracture toughness.

- Assess localised constraint effects found in geometries with complex defect shapes.

- Make adjustments to fracture toughness values based on specimen and defect geometry, material properties and local constraint (leading to considerable variation in the effective crack driving force around a crack front).

- Provide improved understanding of the likely locations of cleavage failure in geometries with complex defects, which is knowledge that could be of use for improvements in in-service testing and evaluation.

Heterogeneity (inhomogeneity) in fracture toughness datasets, in the ductile to brittle transition regime, may occur where there is significant scatter due to a bimodal or a random distribution of particles (e.g. the fracture toughness properties of welds). This cannot be accounted for adequately using the Master Curve methods provided in the standards. Another tool will therefore be developed that aim to:

- Provide simplistic methods for assessing the effects of heterogeneity in fracture toughness datasets.

- Include these methods in a predictive tool, validated against data from the literature. These tools would provide more appropriate (and less conservative) effective fracture toughness values for use in assessment.

- Allow the assessment of the effects of measurement uncertainty on these effective fracture toughness values.

### 3.3 DEVELOPMENT OF A SPECIMEN FOR ASSESSING IN-PLANE CONSTRAINT IN THIN COMPONENTS

The analysis of standard fracture mechanics specimens usually yields high constraint (plane strain) fracture toughness data, which is conservative for use in defect tolerance assessments. In components with small dimensions in the plane of the defect (e.g. small ligaments or small widths), the in-plane constraint is thought to potentially have a significant effect on the effective fracture toughness of the component.
The objectives of this phase of work are therefore to:

- Assess in-plane constraint loss in different configurations of a proposed thin-width bend specimen.

- Help to inform the debate about the best way to incorporate two-parameter fracture mechanics theory into assessments.

- Provide an appreciation of the variability in geometric constraint for bend specimens of different widths, which will be helpful for future assessment of components with similar geometrical characteristics.

- Use cracked-body finite element analysis to investigate the constraint effects in the proposed test specimen, and use data from testing of similar specimens to allow judgements to be made as to the appropriateness of the specimen.

- Confirm the viability or otherwise of a thin-width bend specimen for accurately characterising increases in effective fracture toughness under conditions of low constraint, and understand the transferability of the specimen data to in-service components.

3.4 OUT-OF-PLANE CONSTRAINT EFFECT ON FRACTURE TOUGHNESS

The treatment of out-of-plane constraint loss (i.e. the thickness effect) in defect tolerance assessments is not currently fully understood. Recent studies of the loss of out-of-plane constraint have highlighted that a manipulation of the triaxial stress state could be used to define an out-of-plane constraint parameter, which in turn could be used to describe an increase in apparent fracture toughness. However, the translation of this parameter into a fracture criterion for use in a robust three-parameter fracture mechanics theory currently appears elusive.

The objectives of this phase of work are therefore to:

- Assess the effect on effective fracture toughness of out-of-plane constraint loss in compact tension specimens, and allow an appreciation of the variability in the loss of constraint in the in-plane and out-of-plane directions, which will be helpful for future assessment of components with similar geometrical characteristics.

- Inform future development of test methods, and allow refinements of the methodology for testing thin specimens and interpreting the resulting fracture toughness data.
Use cracked-body finite element analysis to investigate the constraint effects in thin compact tension specimens, and use data from testing of similar specimens to allow judgements to be made as to the appropriateness of the test specimens for yielding useful fracture toughness data.

Assess whether a damage model, based on results from finite element modelling, can be used to predict an increase in fracture toughness in thinner components.

Develop a simple method (such as a scaling equation) for characterising the increase in effective fracture toughness due to a change in thickness for inclusion in the R6 procedure and other standards.

Assess if the specimen is able to accurately characterise increases in effective fracture toughness, and understand the transferability of the fracture toughness data to in-service components.
4. THE COMPANY

4.1 OVERVIEW

Frazer-Nash Consultancy is a systems and engineering technology services company, with a technical heritage going back for a century. The company was formed in 1971 as part of a larger group and was subsequently part of a management buy-out in 1990. In 2007, Frazer-Nash became an autonomous company within Babcock International Group.

Frazer-Nash provide independent, impartial, advice to Government and commercial clients in defence, security, energy, transport and a range of other industries. Maintaining a diverse, balanced business is central to Frazer-Nash's success. At the end of the 2011-2012 financial year, Frazer-Nash employed 442 staff operating from offices in seven cities in the UK, as well as in Adelaide in Australia. Frazer-Nash also routinely deploy staff to customer locations, both on short-term and long-term secondments.

4.2 STRUCTURE

Frazer-Nash is managed by an executive board, which holds overall responsibility for the performance of Frazer-Nash and is accountable to Babcock International Group. The core of the company is organised into a matrix structure, with business and technical axes. The matrix is supported by a range of services in administration, business systems and information technology, contracts, environment, finance, health and safety, human resources, marketing, quality assurance, and security.

The business axis co-ordinates and manages Frazer-Nash's interaction with its marketplaces. The axis is managed by senior business executives, working with business managers who each focus on particular sectors of the market. Business development activity is conducted by the collaboration between business managers and staff from the technical axis.

The majority of Frazer-Nash staff report into the technical axis and provide the expertise which is delivered to its clients. The axis is split into four departments, which is further divided into technical groups each focussed on different areas of technical capability.

The matrix provides a mechanism with which to allocate resources across the full range of the company's activities and with which to balance the business in both the short and the long term.
Technical diversity is encouraged and every member of technical staff has the opportunity to work across a range of markets.

Crucial to the success of the company is the ‘systems approach’ to business. This means that Frazer-Nash uses a structured process to better understand their clients’ requirements and apply the approach to all business processes including marketing, business generation, business delivery and client satisfaction. The systems approach has these key attributes:

- A holistic view of the client’s problem – understanding all facets from the raw technical issues through to the context within which the problem will be solved;
- Method of formulation of the solution – developing an approach to the solution that is appropriate rather than just the easiest, engaging others in wider company skill sets and resources outside of the company;
- Broadening of skills and appreciation of capability – constantly striving to share knowledge of capabilities, and foster internal communications;
- Method of delivery in enquiries and projects – building the systems approach principles into core processes.

Frazer-Nash takes full ownership of client problems and the solutions they provide, utilising the ability to draw on company experience and expertise beyond the immediate team, with a commitment to exceed the client expectations.

Currently, company business is derived from a number of distinct market sectors, mainly: nuclear, power, transport, defence, and marine. Projects for the nuclear industry are a large portion of the business, and a lot of Frazer-Nash staff members are involved in projects concerning the nuclear industry at any given time. The company has decades of experience working in the nuclear industry and gained considerable expertise during this time. Projects for the nuclear industry that are on-going at any time include design, analysis, safety, assurance and programme management for various parts of the industry, including civil power generation, naval nuclear facilities, the nuclear submarine fleet, decommissioning and new build.

4.3 STRATEGIC GOALS

From time to time, the company operates a number of core activities, managed separately from the main business. These initiatives are designed to help stimulate long-term growth of the business. The author of this thesis, in undertaking this EngD, is leading one of these initiatives, developing
fracture mechanics capability within the business, and developing the company image as a technical developer of defect tolerance assessment methodologies, collaborating with academia and other companies in the industry.

Frazer-Nash is a member of the R6 development panel, and as such, provides advice to the panel on developments that could be made to the R6 procedure in the future, as well as assisting with technical activities which are focussed on making sure that the latest developments in fracture mechanics methodology are incorporated into the state of the art procedures for defect tolerance assessment.

The author of this thesis has spent the duration of the EngD working on projects supporting the nuclear industry, with a focus on analysis and assurance of critical components. The focus of this thesis, in developing methods that will be used to make improvements to the R6 procedure, and other methodologies which share its principles, will enable more cost-effective design and accurate analysis of metallic components. The advanced methods are being developed primarily for use with components in the nuclear industry, due to its unique challenges surrounding the degradation of metallic components in harsh environments and complex loading situations. However, the methods will be equally applicable in other industries.

It is envisaged that as a result of the work summarised in this thesis, and undertaken as part of the EngD, that Frazer-Nash will possess a much more important role in the development of activities which seek to improve fracture mechanics methodologies, and will be better placed to assist the nuclear industry in developing more advanced ways of assuring safety of its critical components. The skills and knowledge gained over the course of the EngD will be used in the future to permit the company to identify more ‘systems-like’ approaches to the assessment of defect tolerance, aside from the conventional analyses of defect tolerance that are carried out according to the various codes and standards. Frazer-Nash are at the cutting-edge of research and development in areas such as this, and the research contained in this thesis will provide another platform for further developing this area of the business in the future.
5. PREDICTION OF CLEAVAGE FRACTURE WITH AN ADJUSTED MASTER CURVE METHODOLOGY

5.1 INTRODUCTION

The analysis of fracture toughness test data from standard specimens is often based upon the assumptions of planar crack fronts and homogenous material properties, since this allows for the simplified manipulation of data. However, these assumptions do not hold true for all test geometries or real components.

It was identified that it would be desirable for methods to be developed to allow the statistical adjustment of fracture toughness values obtained from a range of fracture toughness specimen testing. These adjustments could be based on the manipulation of a series of inputs including specimen and crack geometry, material properties, loading and constraint. The methods would be developed from Wallin’s investigations [113, 117] into:

- the application of the Master Curve (MC) methodology to postulated defects in real component geometries, where there can be significant changes in the effective crack driving force around a crack front;
- methods for dealing with material heterogeneity in datasets, e.g. in the treatment of fracture toughness properties of welds.

Data obtained from relevant test programmes identified in the literature were used to help validate the developed methods, and provide an indication of the output that can be obtained.

5.1.1 Adjustments for Local Driving Force Variation

The first tool that was developed allows a comparison of a variation of material fracture toughness throughout a component to a variation of the localised effective crack driving force. For a postulated defect and a given loading configuration, this leads to a probabilistic prediction of the location of fracture initiation and the failure load. The tool was developed using Visual Basic (VBA) macros and user-defined functions within an interactive Microsoft Excel workbook. The computational analysis performed by the tool is based on a series of inputs including the defect geometry, material properties, crack-tip constraint and loading. The tool calculates the variation in
effective crack driving force around the postulated defect and models the variation in fracture
toughness. Appropriate limits of validity are defined and restrictions on the analysis hard-coded
into the tool, to prevent inappropriate conclusions being drawn by the operator.

The local levels of constraint defined by the elastic $T$-stress and crack driving force defined by the
$J$-integral around the crack front are fundamental to the estimation of the effective crack driving
force for fracture initiation for any proposed configuration. Cracked body FEA of three-point bend
(3PB) fracture specimens were therefore carried out to provide hard-coded data for the tool. These
were undertaken for a range of defect geometries and material properties. For configurations with
parameter values between those analysed, interpolation was used to determine intermediate
driving forces. For configurations outside the range of validity of the hard-coded data, the option to
input user-defined data is available to characterise the geometry and effective crack driving forces.

The tool uses a Monte Carlo type analysis at discretised points around the postulated defect to
compare effective crack driving forces to the local value of fracture toughness. Values of fracture
toughness are randomly assigned based on a defined probability distribution. The tool was
designed to be easy to operate, with annotation and pop-up messages to assist the user with
providing appropriate inputs to the analysis. The approach is described in greater detail in
Section 5.4.

5.1.2 Lack of Homogeneity in Fracture Toughness Data

A second tool was created where some of the methods identified by Wallin for use with datasets
with suspected heterogeneity have been developed. The inputs to the tool include fracture
toughness values derived from fracture mechanics testing, individual geometrical and material
parameters, as well as any associated measurement of uncertainty. Outputs include the $T_0$ values
(and associated uncertainties) based on the standard SINTAP procedure [111], and the modified
values accounting for any heterogeneity in the dataset. Graphical descriptions of the failure
probability bounds based upon the modified $T_0$ values are presented.

The tool provides indications of the level of heterogeneity in the sample dataset. The modified
values of $T_0$ account for any heterogeneity and are benchmarked against the standard procedure.
The procedure identifies when the standard procedure is still appropriate to use, noting that use of
the standard procedure is desirable in as many cases as possible, for regulatory purposes. The
approach is described in greater detail in Section 5.5.
5.2 BACKGROUND

5.2.1 Standard Master Curve Analysis

A review of the application of the Master Curve (MC) methodology to postulated defects in real components, specimen geometries and heterogeneous datasets was carried out in Section 2.6. A summary of that review is provided here.

Wallin [108] showed that the MC method “enables a complete characterisation of a material’s brittle fracture toughness based on only a few small-size specimens”. This reduces testing costs, whilst improving the quality of lower bound fracture toughness estimates, reducing the need for overly conservative safety factors. The MC method was shown by Wallin [108] to be applicable for practically all steels with a body-centred cubic (BCC) lattice structure, generally identified as ferritic steels. With the MC method, the fracture toughness in the ductile-to-brittle transition (DBT) region is described with a single parameter, the transition temperature, $T_0$ (in °C). This is the temperature at which the median fracture toughness, corresponding to a 25 mm thick fracture mechanics test specimen, is 100 MPa√m. The basic form of the MC method is standardised in the ASTM standard E1921 [109] and $T_0$ values may be derived simplistically using this standard.

The MC reference temperature $T_0$ is obtained from analysis of conventional elastic-plastic fracture mechanics experiments, performed on standard SEN(B) and C(T) specimens having deep notches $(a/W = 0.5)$. The $J$-integral values at cleavage fracture, $J_C$, are derived through the analysis of load-displacement curves measured during the fracture toughness tests.

The test temperature and the configuration of all the specimens should ideally be the same to simplify the data analysis. The test temperature should be selected to be as close as possible to the expected $T_0$. The ASTM standard requires a minimum of six replicate tests which must meet certain criteria relating to specimen size and test temperature.

5.2.2 Effect of Constraint

The interaction of crack-tip plastic zones with nearby traction-free surfaces and with global plastic zones affects the near-tip stresses which control the onset of cleavage fracture. This corresponds to a reduction in the intensity of the crack-tip stress state and a loss of crack-tip constraint which necessitates larger $J$-integral values to trigger cleavage. The $J$-integral becomes invalid on its own as a crack tip characterising parameter when the large strain region reaches a finite size relative to the in-plane dimensions.
The use of plane strain fracture toughness in a fracture assessment is generally considered conservative, since it is conventionally derived from deeply cracked bend specimens using recommended testing standards and validity criteria. These criteria are designed to ensure plane strain conditions and high hydrostatic stresses near the crack tip. The loss of out-of-plane constraint, inherent in thin section components, or the loss of in-plane constraint, perhaps due to shallow cracks or small ligaments, can contribute to increased effective fracture toughness values.

The MC transition temperature, $T_0$, has been related by Wallin [114] to the specimen constraint, expressed in terms of the elastic $T$-stress. The investigation suggested that a linear relationship exists between $T_0$ and the elastic $T$-stress. The relationship was based on analysis of fracture toughness behaviour measured using SEN(B) specimens with varying crack lengths. Studies revealed more subtle differences between deeply cracked SEN(B) and C(T) specimens due to the different $T$-stresses generated by each geometry.

5.2.3 Application of Master Curve Methodology to Realistic Defects

MC parameters are generally determined using test specimens with assumed ‘straight’ crack fronts and a uniform stress state along the crack front. This enables the use of a single $K_I$ value (or an effective $K_J$ value, derived from the applied $J$ integral) and a single constraint value (e.g. a value of $T$-stress) to describe the crack driving force for the whole specimen. For a real crack however, these assumptions are not necessarily valid. Values of $K_I$ (or $K_J$), constraint and temperature can vary along the crack front length, $s$, leading to local discrepancies in $K_I$ (the temperature and specimen size dependent normalisation fracture toughness that corresponds to a 63.2% cumulative failure probability). This leads to the requirement for an adjustment to the cumulative failure probability, to account for an appropriate integral of the relevant parameters over the crack front.

If a defect were to be postulated in a component with material properties and operating conditions which could be analysed using MC methodology, then adjustments could be made to the effective local driving forces around the postulated defect. A probabilistic analysis could therefore be useful to identify the failure driving force around the postulated defect and the likely location of failure.

A modification to Equation 84, to allow identification of the localised effective crack driving force, leads to the simplified equation:
Assessment of the localised effective crack driving forces for a postulated defect for a given loading configuration, may therefore lead to a probabilistic prediction of the location of fracture initiation, for a given variation of fracture toughness through a component, e.g. due to temperature or the attenuation of irradiation embrittlement.

5.2.4 Heterogeneity in Datasets

There can be significant variation in measured fracture toughness values in a given dataset and a significant number of specimen tests may be required to ensure a statistically meaningful measurement. In heterogeneous datasets, there may be additional scatter in fracture toughness values which is beyond that usually expected in a homogeneous dataset.

The SINTAP method [110], as incorporated in the ASTM standard E1921 [109], provides a method to define a lower bound of fracture toughness based on a number of small data sets. The method gives an estimate of the transition temperature (as described in the standard procedure) and then iteratively adjusts this estimate for undue influence of outlier values in the upper tail of the distribution. The method is not useful for separating out the individual constituents of a material with different $T_0$ values. It does not provide an estimate of fracture toughness for the tougher or weaker constituents of the material. Instead, it stops significantly high fracture toughness values unduly affecting the derived $T_0$ value. The lowest fracture toughness (highest $T_0$ value) is also monitored, to assess whether it is significantly different from the $T_0$ calculated for the entire dataset.

The ‘SINTAP Lower Tail’ analysis method is intended for macroscopically homogeneous materials. In reality, ferritic steels are not homogeneous and the fracture toughness properties may depend on the specimen location in the sample. These heterogeneities may be associated with welds, heat affected zones (HAZ) or local carbide distributions. The MC approach has therefore been further developed to enable the analysis of heterogeneous data sets. The algorithms are applicable for both bimodal heterogeneities as well as random heterogeneities.

The bimodal MC method allows a dataset with two distinct populations (e.g. material constituents), to have $T_0$ values determined for each. The method is useful for situations such as the analysis of welded components. The probability of sampling each population can be established along with the individual uncertainties.
The random heterogeneity MC methods can be used to describe a data population for a collection of several materials, or for a distribution of heterogeneities within a material. In a randomly heterogeneous material, \( T_0 \) is assumed to follow a Gaussian distribution characterised by a mean \( T_0 \) and a standard deviation \( \sigma T_0 \). There are two main methods for estimating the distribution – the maximum likelihood (MML) method, which is the more sophisticated method, and the single point estimation (SP) method intended for quick engineering assessment. The SP method gives a simpler estimate of the \( T_0 \) value than is derived through the MML estimation, but it is not as accurate. For small datasets, the MML method is preferable.

### 5.3 FINITE ELEMENT MODELLING APPROACH

#### 5.3.1 Overview

The levels of constraint and \( J \)-integral values around the crack front are fundamental to the estimation of the crack driving force for any proposed configuration. Therefore, 3D cracked body FEA of 3PB fracture mechanics specimens, with a range of defect geometries and material properties, was carried out to provide hard-coded data for the prediction tool. The FE modelling and analysis was undertaken using Abaqus Version 6.9-2 [151]. The results of these analyses are used in the prediction of failure for these types of loading configuration.

#### 5.3.2 Crack Tip Modelling

In FE modelling, sharp cracks are usually modelled using small-strain assumptions. Focused meshes should normally be used for small-strain fracture mechanics evaluations. For a sharp crack the strain field becomes singular at the crack tip. Generally, the mesh design should take account of the singularity at the crack tip in small-strain analysis in Abaqus [151] through the choice of crack tip element type and mesh refinement. Including the singularity often improves the accuracy of the \( J \)-integral, because the calculated stresses and strains in the region close to the crack tip more closely follow the HRR solution under high constraint conditions.

The size of the crack-tip elements also influences the accuracy of the solutions; the smaller the radial and angular dimensions of the elements at the crack tip, the more accurate the stress and strain results will be and, therefore, the more accurate the contour integral calculations will be. According to Abaqus [151], in many cases, if sufficiently fine meshes are used, accurate contour integral values can be obtained without using singular elements.

The crack-tip strain singularity depends on the material model used. Linear elastic, perfectly plastic, and power-law hardening material models are commonly used in FEA for fracture
mechanics models. In Abaqus, the Ramberg-Osgood [36] deformation plasticity model with von Mises yielding behaviour is available. This is implemented in Abaqus with the form described in Equation 13.

The Abaqus finite element code does not model a pure linear elastic region when the deformation plasticity model is used i.e. the material behaviour described by the model in Abaqus is nonlinear at all stress levels, but for commonly used values of the hardening exponent ($n \sim 5$ or more), the nonlinearity only becomes significant for stresses approaching and exceeding $\sigma_0$.

5.3.3 Geometry

The 3PB test specimen is shown in Figure 34. The specimen was modelled in three dimensions to capture through-thickness variations of fracture mechanics parameters and stress fields. Quarter-model meshes were constructed, using planar symmetry about the crack face plane and at the mid-plane in the out-of-plane direction. A standard 25 mm x 50 mm rectangular 3PB specimen with four defect shapes under simple bending loading was chosen.

A standard through-thickness defect with a planar crack front, and three surface defects with semi-elliptical crack fronts (with aspect ratios half-length to depth $c/a = 0.5, 1.0, 2.0$) were modelled. Four crack depths for each of these four defect shapes were chosen. A summary of the dimensions of the various models is presented in Table 1. For configurations with geometrical parameter values between those analysed, interpolation is used in the prediction tool to determine the crack driving forces.

8-noded quadratic elements with reduced integration were used in the analysis (Abaqus element type C3D8R) to reduce computational cost. These would not provide as accurate fracture mechanics parameters at the crack tip as would be generated using 20-noded quadratic elements (which would be able to model the singularity more accurately) however for the purposes for providing reference data for the prediction software, they were considered sufficiently accurate. However, in order to be as accurate as possible, a highly refined and focussed mesh was employed at the position of the crack, with 16 angular elements around the semi-plane. Elements were spaced so that the distance between the contour integrals became geometrically smaller (with a fixed scaling factor on element width of 1.1) towards the crack tip elements (which had a length of $1 \times 10^{-3}$ mm). At the crack tip, collapsed quadrilateral elements were used with coincident nodes at the crack tip merged to a single node for elastic analyses, and coincident nodes permitted to move independently for elastic-plastic analyses.

Each model with a through-thickness planar crack front was meshed using 20 elements through the half-thickness, with the element dimensions decreasing as the free surface was approached.
(allowing stress gradients close to the surface to be accurately calculated). Each model with a surface-breaking semi-elliptical defect was meshed using 20 elements along the crack front, with the element dimensions roughly constant along the crack front.

Figure 39 shows a sample of two of the meshes used in the analyses, with Figure 40 showing a close up of the crack tip area for the meshes.

### 5.3.4 Material Properties

Values of Young’s modulus and Poisson’s ratio for use in the FEA were chosen to be appropriate for steels of interest close to ambient temperature ($E = 200$ GPa, $\nu = 0.3$). The Ramberg-Osgood nonlinear elastic-plastic material model (Equation 13, as described in Section 5.3.2) was used to define the stress-strain curve in these analyses. Two different hardening exponents were assumed ($n = 5, 10$), to bound a range of hardening behaviours for ferritic steels of interest.

The yield stress chosen for the modelling was 450 MPa, which was judged to be a reasonable nominal yield stress for the steels of interest at ambient temperature. It should be noted that across the likely temperature range of interest, material properties would vary from those used in these analyses. However, the properties used are reasonable for the purposes of the prediction tool which includes guidance regarding its limits of validity.

The two Ramberg-Osgood stress-strain curves used in the analyses are presented in Figure 41. Material parameters used in the model are summarised in Table 2.

### 5.3.5 Loads and Boundary Conditions

For the linear elastic analyses, a concentrated nodal force was applied to a reference point, kinematically constrained to all nodes in the model representing the location of the upper test rig rollers (see Figure 42). A nodal force of 200 N distributed across the roller location led to an applied loading at the mid-plane roller of 400 N (due to symmetry).

For the elastic-plastic analyses, the magnitude of the applied load was uniquely defined for each of the geometries, depending on the calculated limit load. The following solution from R6 Section IV.1.5.2 [4] (using a von Mises formulation) was used to define the limit load for a 3PB specimen with a through-thickness planar defect:

$$ N_L = \frac{n_1 W^2 B \sigma_y}{2S} $$

where $2S$ is the distance between the rollers, and:
For a 3PB specimen with a surface-breaking semi-elliptical defect, no standard limit load solution is available, so the limit load was based upon the solution for a through-thickness planar defect, with a depth of 5 mm (which is a simple, and conservative approximation). Ten loading steps were defined for each elastic-plastic analysis, in equal increments.

The applied loadings were defined to cover an approximate range of $0 < L_r < 1.5$. This range of loading is adequate to ensure that the fracture mechanics parameters could be derived for loading states up to and beyond the likely failure load of the component.

The models were physically constrained using a symmetric boundary condition on the crack plane along the uncracked ligament (preventing in-plane rotation and axial displacement), and also along the mid-plane of the geometry (perpendicular to the crack plane). Vertical constraints were also applied at the location of the mid-plane roller to prevent free body motion. Applied loads and boundary conditions are shown in Figure 42.

The direction of the initiation of cracking for this geometry was assumed to be along the crack plane, since the geometry and loading is symmetrical. Crack tip parameters ($J$-integral and $T$-stress) were therefore extracted, using the domain integral method in Abaqus, along this virtual crack extension direction. The parameters were extracted along 20 contours extending radially out from the crack tip, along all available nodal points extending along the crack front. This allowed the variation in fracture mechanics parameters extending radially out from the crack tip to be studied. It is noted that the first two contour integrals extending radially out from the crack tip, in addition to contour integral values at free surfaces, were considered to be inaccurate in providing appropriate data and were therefore excluded.

### 5.3.6 FE Modelling Results

#### 5.3.6.1 Linear Elastic Modelling

This section describes results obtained for an applied 400 N load, but can be scaled linearly.

Figure 43 and Figure 44 show the variation of $J$-integral and $T$-stress across the contour integrals (at the mid-plane and free surface), for the 20 mm deep planar crack front. These figures illustrate

\[
n_L = \frac{2}{\sqrt{3}} \left[ 1.12 + 1.131 \frac{a}{W} - 3.194 \left( \frac{a}{W} \right)^2 \left( 1 - \frac{a}{W} \right)^2 \right] \quad \text{for} \quad 0 \leq \frac{a}{W} \leq 0.18
\]

\[
n_L = \frac{2}{\sqrt{3}} \left[ 1.22 \left( 1 - \frac{a}{W} \right)^2 \right] \quad \text{for} \quad 0.18 \leq \frac{a}{W} \leq 1
\]
the contour independence for the $J$-integral values (aside from the first two contours) and some contour dependence for the $T$-stress values. This behaviour is consistent for the other planar crack front geometries. The contour dependence for the $T$-stress values is due to the fact that 8-noded elements were used (which cannot accurately predict the crack tip parameters and stress gradients close to the crack tip as accurately as quadratic elements). However, at a small distance from the crack tip (approximately 0.1 mm), the $T$-stress values obtained at the different contour integrals converge.

Figure 45 and Figure 46 show the variation of $J$-integral and $T$-stress across the contour integrals (along the crack front), for the geometry with the surface-breaking semi-elliptical crack front ($a = 5$ mm, $c = 5$ mm). These figures illustrate the contour independence for the $J$-integral values (aside from the first two contours) and some contour dependence for the $T$-stress values (similar to that for the planar defects). This behaviour is consistent for the other semi-elliptical crack front geometries.

Figure 47 shows the variation of $J$-integral across the specimen thickness (at the fifth contour integral), for the specimen with a through-thickness planar defect, for the different crack depths studied. Figure 48 shows the variation of $T$-stress (converged values, at the 40th contour, 0.34 mm from the crack tip) across the specimen thickness, for the different crack depths studied.

Figure 49 shows the variation of $J$-integral across the crack front (at the fifth contour integral), for the specimen with a surface-breaking semi-elliptical defect, for the different crack geometries studied. Figure 50 shows the variation of $T$-stress (converged values, at the 20th contour, 0.07 mm from the crack tip) across the crack front, for the different crack geometries studied. The choice of the 40th or 20th contour for $T$-stress was necessary to obtain converged values, as linear elements are not as accurate as quadratic elements in the calculation of $T$-stress, however as stated previously, the $T$-stress data to be used in the prediction tool is for the purposes for providing reference data for the prediction software, and will therefore be appropriate.

These figures show the effect of the free surfaces on the $T$-stress, and the importance of analysing contour integral values across the crack front as well as radially from the crack tip, when determining contour values with path independence.

Figure 51 shows the variation of elastic SIF with crack depth, for the specimen with a through-thickness planar defect. The SIF was calculated as a weighted average of the through-thickness values (based on the fifth contour integral), excluding the surface element contour values. Figure 51 also includes the expected results based upon the relevant SIF solution.
from R6 Section IV.3.6.5 [4], for a three-point bend specimen (with an \( S/W \) ratio of 4), at different crack depths:

\[
K_I = \frac{3FS}{2BW^2} f\left(\frac{a}{W}\right)\sqrt{\pi a}
\]

where \( F \) is the applied force, and:

\[
f\left(\frac{a}{W}\right) = \frac{1.99 - \left(\frac{a}{W}\right)\left(1 - \frac{a}{W}\right)\left[2.15 - 3.93\left(\frac{a}{W}\right) + 2.7\left(\frac{a}{W}\right)^2\right]}{\sqrt{\pi} \left(1 + \frac{2a}{W}\left(1 - \frac{a}{W}\right)^{3/2}\right)}
\]

It is noted that the FE predicted values agree well (within ~4%) with those provided in R6 [4] Section IV.3.6.5. This gives confidence that the FE mesh is refined sufficiently to be able to calculate the \( T \)-stress parameter.

Figure 52 shows the variation of \( T \)-stress with crack depth, for the specimen with a through-thickness planar defect. The \( T \)-stress was calculated at the mid-plane. Figure 52 also includes the expected results based upon a solution obtained by Sham [152] summarised by Sherry et al. [56], for a three-point bend specimen (with an \( S/W \) ratio of 3):

\[
T = \frac{3FS}{2BW^2} \left[0.111 - 8.982\left(\frac{a}{W}\right) + 53.61\left(\frac{a}{W}\right)^2 - 109.32\left(\frac{a}{W}\right)^3 + 78.977\left(\frac{a}{W}\right)^4\right]
\]

The trend of FE predicted values is seen to be similar to those based on the Sham [152] solution, although there are some small differences due to the differing \( S/W \) ratios assumed. This level of agreement provides confidence in the models developed for subsequent analyses.

Table 3 summarises selected crack tip parameters obtained for the linear elastic models (at the mid-plane for the planar crack front geometries, and at the deepest point for the semi-elliptical crack front geometries).

### 5.3.6.2 Elastic-Plastic Modelling

Figure 53 shows the variation of \( J \)-integral (normalised by the mid-plane value) with increasing applied load, around the crack front, for a sample geometry with a semi-elliptical surface defect \((a = 5\text{ mm}, c = 5\text{ mm})\). This plot shows how the maximum \( J \)-integral is usually found near the
surface point of the defect, however as the load increases, the deepest point $J$-integral approaches the near surface value, and finally surpasses it. However the largest $J$-integral around the crack front under all applied loads is found near to the surface point of the defect. The $J$-integral profile around the crack front is similar for other geometries.

Figure 54 shows the variation of $J$-integral with applied load, at the deepest point and at the surface point for the above geometry. For an $L_r$ value up to about 0.6, the surface point $J$ integral value is greater than the deepest point value. Above this $L_r$ value, the deepest point $J$ integral value is greater. The load versus $J$-integral relationship is similar under all geometries and configurations.

5.3.7 Summary

The levels of constraint and $J$-integral values around the crack front for a variety of defect geometries and material properties have been determined using 3D cracked body FEA. These fracture mechanics parameters will be used in the prediction tool to be described in the following section.

5.4 PREDICTION TOOL – DRIVING FORCE ADJUSTMENT

5.4.1 Objectives

The prediction tool was developed to assess the critical loads for cleavage fracture initiation for a range of defects. These predictions are based on a series of user inputs that define defect geometry, crack driving forces, and material properties within defined ranges of validity. Data from the FEA described in the previous section are hard-coded into the tool to provide the basis for predictions of failure for structural components containing similar defect geometries.

In the prediction tool, a Monte Carlo type analysis is used to compare effective crack driving forces at discretised points around the postulated defect to the local value of fracture toughness. The values of fracture toughness are calculated from the transition temperature $T_0$ value, which is randomly assigned based on a prescribed normal distribution curve. Constant values were assumed for yield stress, Young’s modulus, and Poisson’s ratio (i.e. those used in the FE, see Table 2). The tool was designed to be easy to operate, with annotation and pop-up messages to assist the user with providing appropriate inputs to the analysis.
The objectives of this tool are to help understand the likely locations of cleavage failure in components with unusual defect geometries; enabling the analyst to concentrate non-destructive evaluation effort on the more critical areas of the defective component, or to make modifications to the loading regime such that the burden is more equally shared amongst regions of a component with postulated defectiveness which are less likely to be the initiating point for any fracture. The prediction tool will also assist with making adjustments to the calculated failure driving forces and effective fracture toughness values in these components (reducing conservatisms in defect tolerance assessments, and leading to more cost-effective design).

A flow-chart (see Figure 55) is provided with the tool, to allow the user to understand the processes as they are being implemented and to act as a guide. A snapshot of the ‘Inputs’ sheet is shown in Figure 56. A description of the operation of the tool (and a user guide) is provided in Appendix A. VBA macros and user-defined functions coded into the tool are provided in Appendix B.

5.4.2 Example Outputs

A sample of the output provided in the ‘Printout’ sheet is shown in Figure 57.

Graphs are produced of the $K_J$ (or effective SIF), $T$-stress and effective crack driving force along the crack front, sampled at the end of the last iteration analysed. A graph of the mean fracture toughness variation with temperature is produced, along with a view of how the fracture toughness varied across the crack front (noting that this is for a single iteration of the analysis – the crack front variation of fracture toughness is re-initialised with each iteration of the analysis). A plot of the number of failures per discretised location is superimposed onto the crack front shape.

The mean and standard deviation of the values of failure load, failure $K_J$ (or effective SIF), and effective crack driving force are calculated. The proportion of brittle/ductile/plastic collapse failures is calculated. A cumulative distribution of failure is generated based on the applied load. The $3\sigma$ value of failure load ($\sim 0.1\%$) is also calculated.

The outputs of most interest are the mean failure driving force and the Monte Carlo distribution of predicted failure locations along the crack front, and probabilistic distribution of failure loads in each case.

For the hard-coded geometries a few example simulations were performed, using a lower bound fracture toughness of 62.2 MPa m$^{-1}$ (based on a $T_0$ value of -50°C and temperature of -50°C), a standard deviation on the $T_0$ value of 5°C, $n = 5$, a Wallin constraint factor of 12 based on the analyses of Wallin [115], and 200 Monte Carlo iterations.
Figure 58 to Figure 60 show the predicted cleavage initiation locations for a sample of the different planar crack front geometries ($a = 5$ mm, $10$ mm, and $30$ mm). The failure driving forces (mean and standard deviation values) are also quoted. It is observed that in general, the location of cleavage failure is more likely to be closer to the mid-plane, where the driving force is higher. At the free surface, where constraint is a lot lower, the likelihood of cleavage failure is much lower.

Figure 61 to Figure 63 show the predicted cleavage initiation locations along a sample of the different semi-elliptical crack fronts studied ($a = 2$ mm and $c = 4$ mm, $a = 3$ mm and $c = 3$ mm, and $a = 5$ mm and $c = 2.5$ mm). The failure driving forces (mean and standard deviation values) are also quoted. It is observed that in general, the location of cleavage failure is more likely to be closer to the deepest point in high aspect ratio defects, and closer to the surface point in lower aspect ratio defects, due to the change in effective crack driving forces around the crack front. The shape of semi-elliptical surface defects has a significant effect on the crack tip constraint and the subsequent effective fracture toughness.

The mean failure $K_J$ (or effective SIF) varies significantly between the different analysed geometries (due to the varying amounts of crack tip constraint). This implies that the effective fracture toughness would be different in each of these cases. This effect and the implications for improvements in estimation of fracture toughness are discussed later (see Section 5.6.1).

5.5 PREDICTION TOOL – HETEROGENEITY

5.5.1 Objectives

The main objectives of this tool are (i) to provide a rigorous methodology for the manipulation of fracture toughness test data from various test conditions and (ii) to identify and account for any heterogeneity in the identification of $T_0$. It is noted that this may yield worse $T_0$ values than derived from the standard procedure but they are likely to be more accurate for a dataset derived from a heterogeneous material.

This tool will provide less conservative $T_0$ values for use in defect tolerance assessments leading to more cost-effective design of future components, and less onerous treatment of in-service components. The tool will also allow the analyst to probabilistically assess the effect of measurement uncertainty on the obtained $T_0$ values – providing a method for identifying where effort should be spent in removing measurement uncertainty.
5.5.2 Methodology

The methods developed in this phase of work are intended to yield estimates of fracture toughness for any given specimen, using the following inputs by the user:

- A fracture toughness calculated using a standard test methodology, e.g. ASTM E1921 [109];
- The specimen geometry;
- Elastic and tensile properties of the material under test;
- The test temperature.

The outputs from the tool include:

- Values of $T_0$ which can be used to characterise the test series for a set of homogenous specimens;
- Values of $T_0$ characterising specimens with discrete bimodal heterogeneity (e.g. HAZ/weld). The probability of these fracture toughness values will be that which characterises the failure for any given specimen. An estimate of the $T_0$ value corresponding to the combined data is also provided;
- For specimens with random heterogeneity, a Gaussian distribution of $T_0$ values;
- Plots of the datasets against the calculated survival probability bounds;
- A histogram for each data set showing the predicted values of $T_0$ versus the expected values using the basic SINTAP methodology, as a visual measure of the heterogeneity;
- The applicability of the methods for a given population.

5.5.3 Operation

Operation of the prediction tool is performed in stages. A summary is provided here:

- Input of the details of the test specimen geometry, material properties and test parameters. Input of the test temperatures and fracture toughness values (either manually derived from the tests, or using an automatic dataset generator);
- Derivation of the ‘SINTAP Lower Tail’ analysis estimates of $T_0$. An indication of whether there is any likelihood of significant heterogeneity is provided;

- Derivation of $T_0$ values assuming a bimodal distribution of fracture toughness values in the population. An indication of whether there is any likelihood of significant heterogeneity is provided here. If a bimodal estimate for the population is considered inappropriate, then this is indicated. A summary of these calculations is provided in Section 2.6.4;

- Derivation of $T_0$ values assuming a Gaussian distribution of fracture toughness values in the population. An indication of whether there is any likelihood of significant heterogeneity is provided here. An estimate of the distribution is made using the Single Point Estimate method for reference. An estimate is then made using the Maximum Likelihood model – if the MML model does not yield an appropriate solution, then it is likely that the material is either very homogenous, in which case the SINTAP estimate will suffice, or the variance in the distribution is too large for the tool to deal with. A summary of these calculations is provided in Section 2.6.5;

- Graphs are plotted of the datasets against the calculated survival probability bounds, based on the $T_0$ values derived using the different methods;

- Histograms are plotted of the $T_0$ values from a sample of the population for comparison against the $T_0$ values that would be expected using the SINTAP analysis for the individual analysis;

- Sensitivity studies looking at changes in uncertainty in the various parameters should be performed. The tool can be used to identify the variability in the predicted $T_0$.

A flow-chart (see Figure 64) is included with the on-screen documentation of the tool, to allow the user to understand the processes as they are being implemented and to act as a guide. A snapshot of the inputs area of the tool is shown in Figure 65.

A description of the operation of the tool (and a user guide) is provided in Appendix C. VBA macros and user-defined functions coded into the tool are provided in Appendix D.

### 5.5.4 Automatic Dataset Testing

The methods incorporated within the tool were validated through the use of validation datasets with defined characteristics. Additional validation datasets may be created from within the tool by the user, or real fracture toughness populations with known characteristics may be pasted into the ‘Inputs’ area of the tool.
All sample outputs provided here demonstrate that the models adequately describe the data and provide useful information regarding the predicted uncertainty using each model.

### 5.5.4.1 Example 1 – Homogenous Dataset

A homogenous dataset of 100 test results was generated, with a mean fracture toughness value of 150 MPa$\sqrt{\text{m}}$ and standard deviation of 25 MPa$\sqrt{\text{m}}$, at a test temperature of 0°C with a standard deviation of 1°C.

Parameters output from the tool are presented in Table 4 and plots presented in Figure 66 to Figure 71 for the outputs of the three different analyses (‘SINTAP Lower Tail’ Analysis, Bimodal Heterogeneity Analysis, and Random Heterogeneity (MML Model) Analysis). It is noted that all three analyses yield similar $T_o$ values (-28°C), with small calculated uncertainty values, and that this demonstrates that all methods are appropriate for characterising homogeneous datasets.

### 5.5.4.2 Example 2 – Bimodal Dataset

A dataset of 100 test results was generated with a bimodal distribution. Distribution A had a mean fracture toughness value of 175 MPa$\sqrt{\text{m}}$ and standard deviation of 5 MPa$\sqrt{\text{m}}$ at a test temperature of -25°C with a standard deviation of 2°C. Distribution B had a mean fracture toughness value of 100 MPa$\sqrt{\text{m}}$ and standard deviation of 15 MPa$\sqrt{\text{m}}$ at a test temperature of +25°C with a standard deviation of 2°C. The probability of a datum appearing in Distribution A was 0.4.

Parameters output from the tool are presented in Table 5 and plots presented in Figure 72 to Figure 77 for the outputs of the three different analyses. It is noted that all three analyses yield different $T_o$ values for the dataset (14.1°C for the standard SINTAP analysis, 28.8°C/-58.9°C for the bimodal heterogeneity analysis and -16°C for the random heterogeneity analysis), highlighting the requirement for the output to be studied carefully for datasets with bimodal heterogeneity.

### 5.5.4.3 Example 3 – Dataset with Large Amounts of Scatter

A dataset of 100 test results was generated, with a mean fracture toughness value of 250 MPa$\sqrt{\text{m}}$ and standard deviation of 50 MPa$\sqrt{\text{m}}$ at a test temperature of 0°C with a standard deviation of 25°C. The cumulative probability of fracture toughness and temperature curves for this population are shown in Figure 78 and Figure 79 respectively.

Parameters output from the tool are presented in Table 6 and plots presented in Figure 80 to Figure 85 for the outputs of the three different analyses. It is noted that all three analyses yield different $T_o$ values for the dataset (-58.6°C for the standard SINTAP analysis, -53.0°C/+85.2°C for the bimodal heterogeneity analysis and -62°C for the random heterogeneity analysis). However, a
feel for the degree of heterogeneity can be obtained by observing that the estimate using random heterogeneity analysis is similar to that obtained using the standard SINTAP analysis.

### 5.5.5 Summary

This tool provides the user with a rigorous methodology for the manipulation of fracture toughness test data from various test conditions and allows the identification of any heterogeneity in the calculation of $T_0$. This will provide less conservative $T_0$ values for use in defect tolerance assessments leading to more cost-effective design of future components, and less onerous treatment of in-service components.

The tool also allows the user to probabilistically assess the effect of measurement uncertainty on the obtained $T_0$ values – providing a method for identifying where effort should be spent in removing measurement uncertainty.

### 5.6 DISCUSSION

#### 5.6.1 Comparison with Standard Approaches and Datasets from the Literature

##### 5.6.1.1 Driving Force Adjustment Tool

Fracture toughness data for components with unusual defect shapes (and subsequent levels of constraint) in the literature are scarce, since test specimens are generally based on well understood geometries with planar crack fronts and high constraint conditions, to facilitate calculation of a fracture toughness value.

However, analysis of so-called ‘POR’ specimens of 22NiMoCr37 steel was carried out by Keim [153]. These were regular compact tension specimens, with a semi-elliptical surface crack (approximate depth of 6 mm and a length of approximately 16 mm). This specimen is shown in Figure 86. It was found through analysis of the specimens that the $T_0$ value for the POR specimens (shown in Figure 87) was actually 17°C lower than for the standard compact tension specimens with a planar crack front (shown in Figure 88), indicating loss of constraint, and higher effective fracture toughness. This is similar to the loss of constraint and subsequent increase in effective fracture toughness observed in this study, when comparing bend specimens with planar crack fronts to those with semi-elliptical surface defects.
Additionally, a comparison may be made between the value of the effective fracture toughness at failure as predicted by the analysis, and the increase in apparent fracture toughness that would be obtained through the conventional constraint-modified fracture toughness approach of Ainsworth and O’Dowd [147], summarised in R6 Section III.7.5.3. Both these approaches aim to model the enhancement in the capacity of a component to withstand a load prior to fracture.

As observed in Section 5.4.2, the failure crack driving force increases in planar crack front specimens with shallower cracks, or semi-elliptical surface cracks, due to the reduction in constraint (characterised by a reduction in $T$ stress). This translates to an increased apparent fracture toughness that would be observed in a fracture toughness test of the geometry in question.

Using R6 Section III.7.5.3, the influence of constraint on the material resistance to fracture can be evaluated using the following:

$$K_{mat}^c = K_{mat} \left[ 1 + \alpha \left( -\beta L_r \right)^n \right]$$  \hspace{1cm} (103)

where $\alpha$ and $k$ are material dependent constants. Sherry et al. [149] provide values for $\alpha$ and $k$ in lookup tables, for different values of $n$ and $E/\sigma_y$, relevant to different values of $m$, the Beremin cleavage fracture model parameter for the material.

In this analysis, a value of $E/\sigma_y$ of ~450 is used, and a value for $n = 5$ is assumed. A series of $\alpha$ and $k$ values are extracted from the lookup tables, shown in Table 7. Curves (for the different $m$ values) can then be produced according to Equation 103, for three different values of $K_{mat}$, where the $\beta L_r$ term is equivalent to the normalised $T$-stress ($T/\sigma_y$). The effective fracture toughness versus normalised $T$-stress points at failure were then derived based on the current analysis (for the various analysed geometries). The comparisons are shown in the same figures as the curves, Figure 89 to Figure 91. These figures show that the trends in increasing fracture toughness with reducing constraint are comparable for a constraint-corrected fracture toughness curve with $m = 10$, with more similarity for lower absolute values of $T/\sigma_y$. The deviation for higher absolute values of $T$-stress is due to increased plasticity.

Coupled with the primary objective of the analysis to determine the likelihood of cleavage initiation, the current analysis therefore allows an increase in apparent fracture toughness with reduction in constraint to be studied without reference to the lookup tables, where the Beremin $m$ value may not be known.
5.6.1.2 Heterogeneity Prediction Tool

One of the largest fracture toughness datasets on ferritic material in the DBT transition region is the ‘EURO dataset’ as summarised by Lucon and Scibetta [154]. This dataset was the outcome of a EU-sponsored project involving ten European laboratories in the 1990s, summarised by Heerens and Hellman [155]. More than 700 compact tension specimens of different thickness were tested at different temperatures to produce a large dataset for validation of various statistical methods. This dataset was originally analysed by Heerens and Hellman [156].

The ‘EURO’ material is a large forged, quenched and tempered ring segment of RPV steel 22NiMoCr37, similar to steel class A508 Cl.3. The chemical composition of this steel (in wt%) is shown in Table 8. All of the specimens were extracted from a portion of the plate which was originally considered to be homogenous. This was then divided into several sub-plates, as shown in Figure 92.

The test matrix included tests performed at eight different temperatures from -154°C to 20°C, covering a range from the lower to upper shelf of fracture toughness. Fracture mechanics specimens were standard C(T) specimens with thicknesses ranging from 12.5 mm to 100mm, with $0.52 \leq a/W \leq 0.60$. Most of the specimens were plane-sided. The original analysis suggested that the ‘SX9’ block of material (shown in Figure 92), had a much higher degree of inhomogeneity than the rest of the block.

Lucon and Scibetta [154] characterised this dataset, using the ASTM E1921 approach (SINTAP Lower Tail Analysis Stage 1), the standard SINTAP lower tail analysis approach, the bimodal heterogeneity approach, and the random heterogeneity approach with the following values.

- **ASTM E1921**, $T_0 = -91.3^\circ C$, $\sigma T_0 = 1.1^\circ C$
- **SINTAP Lower Tail Analysis**, $T_0 = -96.1^\circ C$, $\sigma T_0 = 0.7^\circ C$
- **Bimodal Heterogeneity**, $T_{0A} = -81.6^\circ C$, $\sigma T_{0A} = 1.0^\circ C$, $P_A = 0.91$, $T_{0B} = -110.4^\circ C$, $\sigma T_{0B} = 7.3^\circ C$ (indicating likely heterogeneity)
- **Random Heterogeneity**, $T_0 = -83.0^\circ C$, $\sigma T_0 = 11.4^\circ C$ (indicating likely heterogeneity)

The analysis methods developed in this project yield similar estimates:

- **ASTM E1921**, $T_0 = -88.6^\circ C$, $\sigma T_0 = 4.05^\circ C$
- **SINTAP Lower Tail Analysis**, $T_0 = -78.2^\circ C$, $\sigma T_0 = 4.05^\circ C$ (indication of heterogeneity)
Bimodal Heterogeneity, $T_{0A} = -82.9^\circ C$, $\sigma T_{0A} = 0.9^\circ C$, $p_A = 0.91$, $T_{0B} = -111.3^\circ C$, $\sigma T_{0B} = 2.1^\circ C$ (indicating likely heterogeneity)

Random Heterogeneity, $T_{0} = -85.0^\circ C$, $\sigma T_{0} = 10.0^\circ C$ (indicating likely heterogeneity)

The output from the heterogeneity prediction tool is presented in Figure 93 to Figure 97 for the outputs of the three different analyses ('SINTAP Lower Tail' Analysis, Bimodal Heterogeneity Analysis, and Random Heterogeneity (MML Model) Analysis).

Generally, these estimates are within a few per cent of the Lucon and Scibetta [154] estimates, except for the values of $T_0$ for the 'SINTAP Lower Tail' Analysis. In the Lucon and Scibetta analysis, data at test temperatures which are further than 50°C away from the Stage 1 estimate of $T_0$ are censored. The analysis methods used in this tool do not censor these values automatically, however values at extreme temperatures can be censored manually by the user if desired. In this example, the data at these extreme temperatures are not contrary to values expected based on the calculated Master Curve, and so they were not excluded from the analysis. An additional difference is that the Lucon and Scibetta [154] estimates use a slightly different method of data censoring based on the $K_{JC(limit)}$ value than is recommended in the current ASTM E1921 approach.

It is clear from this comparison that there is a significant effect of the different censoring methods on the final results of the method, and the user of the methods should be aware of the effect of censoring on any given dataset. However, the comparison between these analyses and the Lucon and Scibetta analyses [154] gives confidence that the methods that were developed are accurate.

As a demonstration of the increased functionality of the proposed methods, a measurement uncertainty was given to the different variables in the test data as follows:

- Fracture toughness uncertainty, $1\sigma = 10$ MPa/$\sqrt{m}$
- Test temperature uncertainty, $1\sigma = 1^\circ C$
- Specimen thickness, width and crack depth uncertainty, $1\sigma = 0.01$ mm
- Young’s modulus, $1\sigma = 0.5$ GPa
- Yield stress, $1\sigma = 0.5$ MPa

Including these uncertainties, the analysis methods provide these estimates:

- ASTM E1921, $T_0 = -89.4^\circ C$, $\sigma T_0 = 4.05^\circ C$
- SINTAP Lower Tail Analysis, $T_0 = -78.1^\circ C$, $\sigma T_0 = 4.05^\circ C$ (indication of heterogeneity)

- Bimodal Heterogeneity, $T_{0A} = -83.4^\circ C$, $\sigma T_{0A} = 0.9^\circ C$, $p_A = 0.90$, $T_{0B} = -111.5^\circ C$, $\sigma T_{0B} = 1.9^\circ C$ (indicating likely heterogeneity)

- Random Heterogeneity, $T_0 = -86.0^\circ C$, $\sigma T_0 = 11.0^\circ C$ (indicating likely heterogeneity)

Different estimates may be obtained, if another analysis were to be run under these same conditions, due to the nature of the randomly applied measurement uncertainties. For a distribution of values, a Monte Carlo simulation would need to be performed, where the mean values obtained using a large number of Monte Carlo iterations would be expected to be close to those found using no uncertainties.

### 5.6.2 Technical and Commercial Outcomes

The tools developed as part of this phase of work can be used to:

- Help understand the likely locations of cleavage failure in components with unusual defect geometries; enabling the analyst to concentrate non-destructive evaluation effort on the more critical areas of the defective component, or to make modifications to the loading regime such that the burden is more equally shared amongst regions of a component with postulated defectiveness which are less likely to be the initiating point for any fracture;

- Make adjustments to the calculated failure driving forces and effective fracture toughness values in these components (reducing conservatisms in defect tolerance assessments, and leading to more cost-effective design);

- Probabilistically assess the effect of measurement uncertainty on obtained $T_0$ values – providing a method for identifying where effort should be spent in removing measurement uncertainty;

- Provide a less conservative transition temperature (than that obtained from the standard procedures) for large datasets with significant amounts of heterogeneity;

- Sort disparate fracture toughness populations into bimodal distributions, where the two populations have a likelihood of having similar characteristics.

There are components in-service in industry, which have known patches of defectiveness which after some time, would be too severe to allow the component continued operation, if assessed using the standard methods. These tools allow a much more relaxed approach to the assessment
of defectiveness and provide much less conservative fracture toughness values than would be required in a standard defect tolerance assessment.

5.7 CONCLUSIONS

Two predictive tools have been developed which identify improvements that could be made to the estimation of fracture toughness.

The first predictive tool allows a comparison of a variation of fracture toughness values throughout a component, to a variation of the localised effective crack driving force. For a postulated defect and a given loading configuration, this leads to a probabilistic prediction of the location of fracture initiation, and a less conservative estimate of failure load, which can be used to derive an increased effective fracture toughness for the analysed component. Cracked body finite element analyses of three-point bend fracture specimens were carried out to provide hard-coded data for this tool. These analyses were undertaken for a range of defect geometries and material properties. For configurations with parameter values between those analysed, interpolation is used to determine intermediate driving forces. For configurations outside the range of validity of the hard-coded data, the option to input user-defined data is available to characterise the geometry and effective crack driving forces. This database could be extended to include hard-coded fracture mechanics data for other specimen geometries, crack front shapes and loading configurations.

This tool helps the user to understand the likely locations of cleavage failure in components with unusual defect geometries; enabling non-destructive evaluation effort to be concentrated on the more critical areas of the defective component, or to make modifications to the loading regime such that the burden is more equally shared amongst regions of a component with postulated defectiveness which are less likely to be the initiating point for any fracture.

The prediction tool also allows revisions to be made to the failure driving forces and effective fracture toughness values for these components. These developments will reduce conservatism in defect tolerance assessments, and lead to a more cost-effective design of components in the future.

A review of heterogeneity in datasets and their application to the calculation of more representative fracture toughness values has identified that there are simple methods which may provide more accurate and potentially less conservative $T_0$ values than those derived using the methods within the standard. These methods were incorporated into a second tool, which provides calculation of less conservative $T_0$ values given a provided fracture toughness dataset. The modified values account for any heterogeneity and are benchmarked against the standard procedure.
This tool provides the user with a rigorous methodology for the manipulation of fracture toughness test data from various test conditions and allows the identification of any heterogeneity in the calculation of $T_0$. The tool also allows the user to probabilistically assess the effect of measurement uncertainty on the obtained $T_0$ values – providing a method for identifying where effort should be spent in removing measurement uncertainty.

The prediction tools are designed to be of use only for components made of ferritic steels, which operate at temperatures across the ductile-to-brittle transition region of fracture toughness. The methods incorporated within the tools were compared to methods in the literature, and validated through the use of validation datasets with defined characteristics and example datasets from the literature.

### 5.8 SUGGESTED FUTURE WORK

#### 5.8.1 Driving Force Adjustment Tool

Further developments to the prediction tool and supporting FE analyses could include:

- Additional hard-coded fracture mechanics data for different specimen geometries, crack front shapes and loading configurations.

- Allowing elastic-plastic $J$-integral values to be input for a user-defined geometry.

- Allowing analysis of combined loading (e.g. pressure, bending and tension for a cylinder with a surface defect).

- Inclusion of an adjustment to the predicted fracture initiation load to account for the interaction between proximity to fracture and proximity to plastic collapse.

- Modifications to allow for the variation of temperature for the main material properties used in the analysis (Young's modulus and yield strength).

- Development of the treatment of the $T$-stress correction to make it more relevant to the elastic-plastic analysis, or inclusion of the elastic-plastic $Q$ parameter.

- Inclusion of the effects of out-of-plane constraint loss.

- Investigation into the variation of local tensile properties on the crack driving forces.
5.8.2 Heterogeneity Prediction Tool

Various suggestions are made below for improvements that could be made to the heterogeneity prediction tool in future. These could enhance its functionality and accuracy in the estimation of fracture toughness:

- Treatment of significant amounts of ductile crack growth prior to cleavage fracture.
- Consideration of pre-loading effects on test specimens (such as warm pre-stressing).
- Inclusion of a modification to $T_0$ to account for crack arrest behaviour.
- Development of the histogram outputs to identify distinct populations in the data.
- Treatment of a larger number of distinct populations (e.g. tri-modal distribution).

Some of these suggestions would be more difficult to implement than others, and the benefit that would gained from each would vary depending upon the types of analyses that would be of interest.
### Through-Thickness Planar Defect

<table>
<thead>
<tr>
<th>$a$ (mm)</th>
<th>$a/W$</th>
<th>Limit Load (kN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.1</td>
<td>237.0</td>
</tr>
<tr>
<td>10</td>
<td>0.2</td>
<td>190.2</td>
</tr>
<tr>
<td>20</td>
<td>0.4</td>
<td>107.0</td>
</tr>
<tr>
<td>30</td>
<td>0.6</td>
<td>47.5</td>
</tr>
</tbody>
</table>

### Semi-Elliptical Surface Defect

<table>
<thead>
<tr>
<th>$a$ (mm)</th>
<th>$c/a$</th>
<th>$c$ (mm)</th>
<th>Limit Load (kN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.5</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.5</td>
<td>1.5</td>
<td>237.0</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.5</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>10</td>
<td></td>
</tr>
</tbody>
</table>

**Note** – Limit load for the geometries with semi-elliptical surface defects are based upon the limit load for the standard 3PB specimen with a 5 mm deep through-thickness planar defect.

**Table 1 : Defect Geometries Chosen for FE Modelling of the Three-Point Bend Specimen**

($B = 25$ mm, $W = 50$ mm)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Modulus (GPa), $E$</td>
<td>200</td>
</tr>
<tr>
<td>Poisson’s Ratio, $\nu$</td>
<td>0.3</td>
</tr>
<tr>
<td>Yield Stress (MPa), $\sigma$</td>
<td>450</td>
</tr>
<tr>
<td>Hardening Exponent, $n$</td>
<td>5, 10</td>
</tr>
<tr>
<td>Yield Offset, $\alpha$</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2: Ramberg-Osgood Parameters

<table>
<thead>
<tr>
<th>Through-Thickness Planar Defect</th>
<th>$a$ (mm)</th>
<th>$a/W$</th>
<th>SIF (MPa$\sqrt{m}$)</th>
<th>$T$-Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5</td>
<td>0.1</td>
<td>0.25</td>
<td>-0.62</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0.2</td>
<td>0.35</td>
<td>-0.36</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.4</td>
<td>0.59</td>
<td>0.18</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>0.6</td>
<td>1.12</td>
<td>1.30</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Semi-Elliptical Surface Defect (at Deepest Point)</th>
<th>$a$ (mm)</th>
<th>$c/a$</th>
<th>$c$ (mm)</th>
<th>SIF (MPa$\sqrt{m}$)</th>
<th>$T$-Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2</td>
<td>0.5</td>
<td>1</td>
<td>0.056</td>
<td>-1.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
<td>2</td>
<td>0.091</td>
<td>-0.85</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0</td>
<td>4</td>
<td>0.122</td>
<td>-0.79</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.5</td>
<td>1.5</td>
<td>0.067</td>
<td>-0.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
<td>3</td>
<td>0.108</td>
<td>-0.79</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0</td>
<td>6</td>
<td>0.147</td>
<td>-0.75</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.5</td>
<td>2</td>
<td>0.074</td>
<td>-0.88</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
<td>4</td>
<td>0.121</td>
<td>-0.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0</td>
<td>8</td>
<td>0.168</td>
<td>-0.68</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>0.5</td>
<td>2.5</td>
<td>0.079</td>
<td>-0.82</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0</td>
<td>5</td>
<td>0.132</td>
<td>-0.66</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0</td>
<td>10</td>
<td>0.189</td>
<td>-0.59</td>
</tr>
</tbody>
</table>

Table 3: Linear Elastic FE Modelling Results (Applied Load of 400 N)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Specimens</td>
<td>100</td>
</tr>
<tr>
<td>Minimum Censoring Limit</td>
<td>383 MPa√m</td>
</tr>
<tr>
<td>Distribution Toughness (Mean / Standard Deviation)</td>
<td>150 MPa√m, 25 MPa√m</td>
</tr>
<tr>
<td>Distribution Temperature (Mean / Standard Deviation)</td>
<td>0°C, 1°C</td>
</tr>
<tr>
<td><strong>SINTAP Lower Tail Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 1)</td>
<td>-27.5°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>4.39°C</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 2)</td>
<td>-27.5°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>4.39°C</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 3)</td>
<td>13.5°C</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Bimodal Heterogeneity Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Estimate for Distribution A</td>
<td>-27.5°C</td>
</tr>
<tr>
<td>$T_0$ Estimate for Distribution B</td>
<td>N/A</td>
</tr>
<tr>
<td>Probability of Fracture Toughness Belonging to Distribution A</td>
<td>1.00</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ Estimate for Distribution A</td>
<td>2.22°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ Estimate for Distribution B</td>
<td>N/A</td>
</tr>
<tr>
<td>Uncertainty on Probability of Fracture Toughness Belonging to Distribution A</td>
<td>0.04</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>No</td>
</tr>
<tr>
<td>$T_0$ Estimate for Combined Population</td>
<td>-27.5°C</td>
</tr>
<tr>
<td><strong>Random Heterogeneity Analysis</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Single Point Estimate</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Mean</td>
<td>-22.5°C</td>
</tr>
<tr>
<td>$T_0$ Standard Deviation</td>
<td>0.01°C</td>
</tr>
<tr>
<td><strong>Maximum Likelihood Estimator</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Mean</td>
<td>-28°C</td>
</tr>
<tr>
<td>$T_0$ Standard Deviation</td>
<td>0°C</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>No</td>
</tr>
</tbody>
</table>

**Table 4**: Output from Validation Performed on Homogeneous Dataset
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Specimens</td>
<td>100</td>
</tr>
<tr>
<td>Minimum Censoring Limit</td>
<td>383 MPa/m</td>
</tr>
<tr>
<td>Distribution A Fracture Toughness (Mean / Standard Deviation)</td>
<td>175 MPa/m, 5 MPa/m</td>
</tr>
<tr>
<td>Distribution A Temperature (Mean / Standard Deviation)</td>
<td>-25°C, 2°C</td>
</tr>
<tr>
<td>Distribution B Fracture Toughness (Mean / Standard Deviation)</td>
<td>100 MPa/m, 15 MPa/m</td>
</tr>
<tr>
<td>Distribution B Temperature (Mean / Standard Deviation)</td>
<td>25°C, 2°C</td>
</tr>
<tr>
<td>Approximate Proportion of Data in Distribution A</td>
<td>0.4</td>
</tr>
<tr>
<td><strong>SINTAP Lower Tail Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 1)</td>
<td>-47.2°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>4.39°C</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 2)</td>
<td>14.1°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>4.39°C</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 3)</td>
<td>65.3°C</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Bimodal Heterogeneity Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Estimate for Distribution A</td>
<td>28.8°C</td>
</tr>
<tr>
<td>$T_0$ Estimate for Distribution B</td>
<td>-58.9°C</td>
</tr>
<tr>
<td>Probability of Fracture Toughness Belonging to Distribution A</td>
<td>0.55</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ Estimate for Distribution A</td>
<td>3.03°C</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ Estimate for Distribution B</td>
<td>2.43°C</td>
</tr>
<tr>
<td>Uncertainty on Probability of Fracture Toughness Belonging to Distribution A</td>
<td>0.05</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>Yes</td>
</tr>
<tr>
<td>$T_0$ Estimate for Combined Population</td>
<td>9.6°C</td>
</tr>
<tr>
<td><strong>Random Heterogeneity Analysis</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Single Point Estimate</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Mean</td>
<td>-2.1°C</td>
</tr>
<tr>
<td>$T_0$ Standard Deviation</td>
<td>50.81°C</td>
</tr>
<tr>
<td><strong>Maximum Likelihood Estimator</strong></td>
<td></td>
</tr>
<tr>
<td>$T_0$ Mean</td>
<td>-16°C</td>
</tr>
<tr>
<td>$T_0$ Standard Deviation</td>
<td>44°C</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Table 5: Output from Validation Performed on Dataset with Bimodal Heterogeneity
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Specimens</td>
<td>100</td>
</tr>
<tr>
<td>Minimum Censoring Limit</td>
<td>383 MPa√m</td>
</tr>
<tr>
<td>Distribution Fracture Toughness (Mean / Standard Deviation)</td>
<td>250 MPa√m, 50 MPa√m</td>
</tr>
<tr>
<td>Distribution Fracture Toughness (Mean / Standard Deviation)</td>
<td>0°C, 25°C</td>
</tr>
</tbody>
</table>

**SINTAP Lower Tail Analysis**

<table>
<thead>
<tr>
<th>$T_0$ Estimate (Stage 1)</th>
<th>$-72.1°C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>$4.39°C$</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 2)</td>
<td>$-58.6°C$</td>
</tr>
<tr>
<td>Uncertainty on $T_0$ (Stage 1)</td>
<td>$4.39°C$</td>
</tr>
<tr>
<td>$T_0$ Estimate (Stage 3)</td>
<td>$21.7°C$</td>
</tr>
<tr>
<td>Indication of Heterogeneity</td>
<td>Yes</td>
</tr>
</tbody>
</table>

**Bimodal Heterogeneity Analysis**

| $T_0$ Estimate for Distribution A | $-53.0°C$                              |
| $T_0$ Estimate for Distribution B | $-85.2°C$                              |
| Probability of Fracture Toughness Belonging to Distribution A | 0.67                                    |
| Uncertainty on $T_0$ Estimate for Distribution A | $2.73°C$                              |
| Uncertainty on $T_0$ Estimate for Distribution B | $2.87°C$                              |
| Uncertainty on Probability of Fracture Toughness Belonging to Distribution A | $0.04$                                 |
| Indication of Heterogeneity | Yes                                     |
| $T_0$ Estimate for Combined Population | $-60.8°C$                             |

**Random Heterogeneity Analysis**

**Single Point Estimate**

| $T_0$ Mean | $-57.0°C$                      |
| $T_0$ Standard Deviation | $16.76°C$                      |

**Maximum Likelihood Estimator**

| $T_0$ Mean   | $-62°C$                      |
| $T_0$ Standard Deviation | $18°C$                      |

Table 6: Output from Validation Performed on Dataset with Random Heterogeneity
<table>
<thead>
<tr>
<th>m</th>
<th>5</th>
<th>7.5</th>
<th>10</th>
<th>12.5</th>
<th>15</th>
<th>17.5</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>0.708</td>
<td>1.013</td>
<td>1.087</td>
<td>1.017</td>
<td>0.889</td>
<td>0.789</td>
<td>0.806</td>
</tr>
<tr>
<td>k</td>
<td>2.13</td>
<td>1.67</td>
<td>1.41</td>
<td>1.30</td>
<td>1.28</td>
<td>1.30</td>
<td>1.29</td>
</tr>
</tbody>
</table>

Table 7: Sample of Material-Dependent Constants for use with the Constraint-Corrected Toughness Approach of Ainsworth and O’Dowd [147]

<table>
<thead>
<tr>
<th>C</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mn</th>
<th>Ni</th>
<th>Cu</th>
<th>Mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.21</td>
<td>0.24</td>
<td>0.003</td>
<td>0.004</td>
<td>0.003</td>
<td>0.82</td>
<td>0.79</td>
<td>0.049</td>
<td>0.56</td>
</tr>
</tbody>
</table>

Table 8: Chemical Composition of 22NiMoCr37 Steel (EURO Dataset) [156]
5.10 FIGURES

Figure 39: View of Two of the Meshes Used in the Modelling
a) Through-Thickness Planar Defect ($a = 20$ mm)

b) Semi-Elliptical Surface Defect ($a = 5$ mm, $c = 5$ mm)

Figure 40: Close-up Views of Crack Tip Meshes
a) Through-Thickness Planar Defect ($a = 20$ mm)

b) Semi-Elliptical Surface Defect ($a = 5$ mm, $c = 5$ mm)
Figure 41: Linear Elastic and Elastic-Plastic Ramberg-Osgood Stress-Strain Curves Used in the FEA

Figure 42: Boundary Conditions in the FEA
Figure 43: Linear-Elastic Analysis – $J$-Integral vs. Contour Number, Mid-Plane and Surface,
Through-Thickness Defect, $a = 20$ mm (400 N Applied Load)

Figure 44: Linear-Elastic Analysis – $T$-Stress vs. Contour Number, Mid-Plane and Surface,
Through-Thickness Defect, $a = 20$ mm (400 N Applied Load)
Figure 45: Linear-Elastic Analysis – $J$-Integral vs. Contour Number, Deepest Point and Surface Point, Semi-Elliptical Defect, $a = 5$ mm, $c = 5$ mm (400 N Applied Load)

Figure 46: Linear-Elastic Analysis – $T$-Stress vs. Contour Number, Semi-Elliptical Defect, $a = 5$ mm, $c = 5$ mm, Deepest Point and Surface Point (400 N Applied Load)
Figure 47: Linear-Elastic Analysis – Variation of $J$-Integral along the Crack Front, Through-Thickness Planar Defect, Different Depths (400 N Applied Load)

Figure 48: Linear-Elastic Analysis – Variation of $T$-Stress along the Crack Front, Through-Thickness Planar Defect, Different Depths (400 N Applied Load)
Figure 49: Linear-Elastic Analysis – Variation of $J$-Integral along the Crack Front, Semi-Elliptical Defect ($a = 5$ mm), Different Aspect Ratios (400 N Applied Load)

Figure 50: Linear-Elastic Analysis – Variation of $T$-Stress along the Crack Front, Semi-Elliptical Defect ($a = 5$ mm), Different Aspect Ratios
Figure 51: SIF vs. Defect Depth, Through-Thickness Planar Defect, 400 N Applied Load
(Comparison with R6 Section IV.3.6.5)

Figure 52: T Stress vs. Defect Depth, Through-Thickness Planar Defect, 400 N Applied Load
(Comparison with solution by Sham [152])
Figure 53: Elastic-Plastic Analysis – Variation of $J$-Integral around Crack for Increasing Loading, Semi-Elliptical Surface Defect ($a = 5$ mm, $c = 5$ mm), $n = 5$

Figure 54: Elastic-Plastic Analysis – Variation of $J$-Integral with Applied Load, Semi-Elliptical Surface Defect ($a = 5$ mm, $c = 5$ mm), $n = 5$
Figure 55: Flow Chart for Operation of the Crack Driving Force Adjustment Tool

**START**
- Specify assessment report name
- Specify mean and standard deviation on $T_n$
- Specify probability distribution on fracture toughness
- Enter the number of calculation iterations
- Enter the assessment temperature
- Enter material model to assess Elastic, Elast-Plastic ($n=5$, or $n=10$)
- Enter the upper shelf fracture toughness (MPa) to predict ductile fractures
- Is a T42 correlation to be applied? (relevant only for planar through-thickness defects)
- Override the Limit Load for a Hard-Coded Geometry?
- Enter a new limit load ($L_H$)

**Inputs Stage Complete**
- Enter a new limit load ($L_H$)
- Elastic and elastoplastic FEA results relevant to the semi-elliptical and planar defects are hard-coded into the tool. These are manipulated to generate effective crack driving forces at positions along the crack front, at each load step in the analysis.
- Click the 'Generate Result' button — this starts the analysis.

**Analysis Complete**
- First iteration complete: repeat process until specified number of iterations is completed
- Details of the failure are recorded (including the failure load, the failure $K_{fc}$, the failure driving force, the classification of failure, and the failure location).
- Plastic collapse has occurred
- Initiation has occurred

**More iterations of calculation required?**
- $A_{T1}$ value is randomly assigned to each discretised point on the crack front, based on the data provided
- A $K_{fc}$ value is then applied to each discretised point, based on the data provided
- The localised crack driving force is calculated
- A load increment is applied.

**Outputs**
- See 'Printout' tab for a summary of the input and analysis data. Graphs of $K_{fc}$, T-stress, and effective crack driving force are provided along the crack front, sampled at the last iteration analysed.
- A graph of mean fracture toughness with temperature is produced, demonstrating the transition region.
- A plot of the number of failures per discretised location is superimposed on the crack front shape.
- The mean and standard deviation of the values of failure load, $K_{fc}$ and effective crack driving force are calculated. The proportion of ductile/plastic collapse failures is calculated.
- A cumulative distribution of failure is generated based on the applied load.
- See report for more information.
Figure 56: Snapshot of the ‘Outputs’ Worksheet in the Prediction Tool

User Defined Inputs For a Load of 1kN

<table>
<thead>
<tr>
<th>Title</th>
<th>Discretised</th>
<th>Point x (mm)</th>
<th>y (mm)</th>
<th>Temp (°C)</th>
<th>J-Integral (N/m)</th>
<th>T-Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T0</td>
<td></td>
<td>0.0</td>
<td>10.0</td>
<td>-50.0</td>
<td>-50.0</td>
<td>10.0</td>
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</tr>
<tr>
<td>T3</td>
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<td>-57.0</td>
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<td>T9</td>
<td></td>
<td>9.0</td>
<td>8.0</td>
<td>-59.0</td>
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<tr>
<td>T10</td>
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<td>-60.0</td>
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<td>-0.5</td>
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<tr>
<td>T11</td>
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<td>11.0</td>
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<td>T15</td>
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<td>-65.0</td>
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<td>-0.6</td>
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<tr>
<td>T16</td>
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<td>10.0</td>
<td>-66.0</td>
<td>10.0</td>
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Mean Toughness Distribution

<table>
<thead>
<tr>
<th>User Name</th>
<th>0.001 Probability Bound (%)</th>
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<tr>
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</tr>
<tr>
<td>7</td>
<td>0.001</td>
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<tr>
<td>8</td>
<td>0.001</td>
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<tr>
<td>9</td>
<td>0.001</td>
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</table>

Temperature (°C)

<table>
<thead>
<tr>
<th>No.</th>
<th>T0</th>
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<th>T0 - standard deviation</th>
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<tbody>
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<td></td>
</tr>
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<td>3</td>
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<td>4</td>
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<td>8</td>
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Ellipse Geometry

<table>
<thead>
<tr>
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<td></td>
</tr>
<tr>
<td>9</td>
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</table>

Material Model

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<tbody>
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<tr>
<td>7</td>
<td></td>
</tr>
<tr>
<td>8</td>
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</tbody>
</table>

Upper Shelf Fracture Toughness (Ductile) (MPa√m)

<table>
<thead>
<tr>
<th>No.</th>
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<tbody>
<tr>
<td>1</td>
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<tr>
<td>2</td>
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<tr>
<td>6</td>
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<tr>
<td>7</td>
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<tr>
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</table>

Depth, a (mm)

<table>
<thead>
<tr>
<th>No.</th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<tr>
<td>7</td>
<td></td>
</tr>
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</table>

Aspect Ratio for Semi-Elliptical Defects (Half Length to Depth)

<table>
<thead>
<tr>
<th>No.</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>120</td>
</tr>
<tr>
<td>2</td>
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<td>4</td>
<td></td>
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<td>5</td>
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<tr>
<td>6</td>
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</tr>
<tr>
<td>7</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
</tr>
</tbody>
</table>
Fracture Initiation Prediction Tool

Test Geometry
Project Number 38194

User Inputs

Material Property Inputs

$T_0$ - Mean: -50 °C
$T_0$ - Standard Deviation: 1 °C

Lower bound toughness

Upper Shelf Toughness (Ductile Failure): 150 MPa m
Ramberg-Osgood Hardening Curve: $n = 5$
Constraint factor: 12

Temperature: -50 °C

Geometry Inputs

Semi-Elliptical Surface Defect
Depth: 5 mm
Aspect Ratio for Semi-Elliptical Defect (Half Length To Depth): 1
Limit Load Assumed: 237.0 kN
T-Stress used in Calculation of Driving Force

Number of Iterations Requested for Analysis: 200

Additional User Comments

Rob Kulka 38194
23-May-11
09:40:56

Figure 57: Snapshot of the ‘Printout’ Worksheet in the Prediction Tool

Page 1 of 4
Figure 57 (continued): Snapshot of the ‘Printout’ Worksheet in the Prediction Tool

Variation of SIF around Crack Front

T-Stress Variation around Crack Front
Figure 57 (continued): Snapshot of the ‘Printout’ Worksheet in the Prediction Tool
Figure 57 (continued): Snapshot of the ‘Printout’ Worksheet in the Prediction Tool
Figure 58: Prediction of Cleavage Initiation Location (Planar Defect, $a = 5$ mm)

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>90.8</td>
<td>2.8</td>
<td>82.4</td>
</tr>
<tr>
<td>Failure SIF (MPa$\sqrt{m}$)</td>
<td>63.9</td>
<td>2.3</td>
<td>57.0</td>
</tr>
<tr>
<td>Effective Driving Force (MPa$\sqrt{m}$)</td>
<td>56.2</td>
<td>1.6</td>
<td>51.3</td>
</tr>
</tbody>
</table>

Figure 59: Prediction of Cleavage Initiation Location (Planar Defect, $a = 10$ mm)

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>61.4</td>
<td>1.5</td>
<td>56.9</td>
</tr>
<tr>
<td>Failure SIF (MPa$\sqrt{m}$)</td>
<td>59.1</td>
<td>1.9</td>
<td>53.2</td>
</tr>
<tr>
<td>Effective Driving Force (MPa$\sqrt{m}$)</td>
<td>56.3</td>
<td>1.7</td>
<td>51.1</td>
</tr>
</tbody>
</table>
Figure 60: Prediction of Cleavage Initiation Location (Planar Defect, $a = 30$ mm)

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>17.0</td>
<td>0.4</td>
<td>15.8</td>
</tr>
<tr>
<td>Failure SIF (MPa√m)</td>
<td>33.8</td>
<td>1.5</td>
<td>49.3</td>
</tr>
<tr>
<td>Effective Driving Force (MPa√m)</td>
<td>56.6</td>
<td>1.7</td>
<td>51.4</td>
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</tbody>
</table>

Figure 61: Prediction of Cleavage Initiation Location (Semi-Elliptical Defect, $a = 2$ mm, $c = 4$ mm)

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>195.1</td>
<td>3.2</td>
<td>185.5</td>
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<tr>
<td>Failure SIF (MPa√m)</td>
<td>120.3</td>
<td>5.5</td>
<td>103.7</td>
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<tr>
<td>Effective Driving Force (MPa√m)</td>
<td>66.4</td>
<td>2.0</td>
<td>60.4</td>
</tr>
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</table>
Figure 62: Prediction of Cleavage Initiation Location (Semi-Elliptical Defect, $a = 3$ mm, $c = 3$ mm)

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>198.9</td>
<td>3.7</td>
<td>187.7</td>
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<td>Failure SIF (MPa·m)</td>
<td>124.6</td>
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<td>105.4</td>
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<td>Effective Driving Force (MPa·m)</td>
<td>66.8</td>
<td>2.2</td>
<td>60.1</td>
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</table>

Figure 63: Prediction of Cleavage Initiation Location (Semi-Elliptical Defect, $a = 5$ mm, $c = 2.5$ mm)

<table>
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<tr>
<th></th>
<th>Mean</th>
<th>St. Dev</th>
<th>3σ Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure Load (kN)</td>
<td>203.6</td>
<td>5.0</td>
<td>188.7</td>
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<tr>
<td>Failure SIF (MPa·m)</td>
<td>143.2</td>
<td>15.8</td>
<td>95.7</td>
</tr>
<tr>
<td>Effective Driving Force (MPa·m)</td>
<td>63.5</td>
<td>2.0</td>
<td>57.5</td>
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</table>
Figure 64: Flow Chart for Operation of the Heterogeneous Dataset Fracture Toughness Prediction Tool
### Figure 65: Sample Input Sheet for the Heterogeneous Fracture Toughness Prediction Tool

<table>
<thead>
<tr>
<th>Description</th>
<th>Option 1</th>
<th>Option 2</th>
<th>Option 3</th>
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<td>OFF</td>
</tr>
<tr>
<td>Property 2</td>
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<td>OFF</td>
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</tr>
<tr>
<td>Property 3</td>
<td>ON</td>
<td>OFF</td>
<td>OFF</td>
</tr>
<tr>
<td>Property 4</td>
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</tr>
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#### Example Data

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<th>Property 5</th>
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</thead>
<tbody>
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<td>Value 1</td>
<td>Value 2</td>
<td>Value 3</td>
<td>Value 4</td>
<td>Value 5</td>
</tr>
</tbody>
</table>

---

**Version 2.0**

Advanced Fracture Toughness Estimation Methods
SINTAP Lower Tail Analysis (Stage 1)

\[ T_0 \text{ Value} = -27.5^\circ C, \quad \text{Uncertainty} = 4.39^\circ C, \quad \text{Potential heterogeneity} = 0.0 \]

![Graph](image1)

Figure 66: Output from Validation Performed on Homogeneous Dataset (From SINTAP Lower Tail Analysis – Stage 1)

SINTAP Lower Tail Analysis (Stage 2)

\[ T_0 \text{ Value} = -27.5^\circ C, \quad \text{Uncertainty} = 4.39^\circ C, \quad \text{Potential heterogeneity} = 0.0 \]

![Graph](image2)

Figure 67: Output from Validation Performed on Homogeneous Dataset (From SINTAP Lower Tail Analysis – Stage 2)
Difference between Expected T0 Values for Individual Tests and Derived T0 Value for Whole Dataset (-27.5°C), Sample of the Population - based upon SINTAP Lower Tail Analysis

Figure 68: Output from Validation Performed on Homogeneous Dataset (From SINTAP Lower Tail Analysis) – Histogram

Bimodal Heterogeneity - Maximum Likelihood Model
There is only one distribution
Distribution A - T0 Value = -27.5°C, Uncertainty = 2.22°C

Figure 69: Output from Validation Performed on Homogeneous Dataset (From Bimodal Heterogeneity Analysis)
Bimodal Heterogeneity - Maximum Likelihood Model
Combined Dataset - T0 Estimate = -27.5°C, Uncertainty = 4.39°C

Random Heterogeneity - Maximum Likelihood Model
Mean T0 Value = -28°C, Standard Deviation = 0°C

Figure 70 : Output from Validation Performed on Homogeneous Dataset (From Bimodal Heterogeneity Analysis – Combined Dataset)

Figure 71 : Output from Validation Performed on Homogeneous Dataset (From Random Heterogeneity Analysis)
**Figure 72**: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From SINTAP Lower Tail Analysis – Stage 1)

**Figure 73**: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From SINTAP Lower Tail Analysis – Stage 2)
Bimodal Heterogeneity - Maximum Likelihood Model
Distribution A - T0 Value = 28.8°C, Uncertainty = 3.03°C,
Distribution B - T0 Value = -58.9°C, Uncertainty = 2.43°C,
Probability of Belonging to Distribution A = 0.55

Figure 74: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From Bimodal Heterogeneity Analysis)

Bimodal Heterogeneity - Maximum Likelihood Model
Combined Dataset - T0 Estimate = 9.6°C, Uncertainty = 4.39°C

Figure 75: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From Bimodal Heterogeneity Analysis– Combined Dataset)
Bimodal Heterogeneity - Maximum Likelihood Model  
Distribution A - $T_0$ Value = 28.8°C, Uncertainty = 3.03°C,  
Distribution B - $T_0$ Value = -58.9°C, Uncertainty = 2.43°C,  
Probability of Belonging to Distribution A = 0.55

Random Heterogeneity - Maximum Likelihood Model  
Mean $T_0$ Value = -16°C, Standard Deviation = 44°C

Figure 76: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From Bimodal Heterogeneity Analysis) – Histogram

Figure 77: Output from Validation Performed on Dataset with Bimodal Heterogeneity (From Random Heterogeneity Analysis)
Figure 78: Output from Validation Performed on Dataset with Random Heterogeneity
(Cumulative Probability of Fracture Toughness Curve)

Figure 79: Output from Validation Performed on Dataset with Random Heterogeneity
(Cumulative Probability of Temperature Curve)
SINTAP Lower Tail Analysis (Stage 1)
T0 Value = -72.1°C, Uncertainty = 4.39°C,
Potential heterogeneity

Figure 80 : Output from Validation Performed on Dataset with Random Heterogeneity (From SINTAP Lower Tail Analysis)

SINTAP Lower Tail Analysis (Stage 2)
T0 Value = -58.6°C, Uncertainty = 4.39°C,
Potential heterogeneity

Figure 81 : Output from Validation Performed on Dataset with Random Heterogeneity (From SINTAP Lower Tail Analysis – Stage 2)
Bimodal Heterogeneity - Maximum Likelihood Model

Distribution A - T0 Value = -53.0°C, Uncertainty = 2.73°C,
Distribution B - T0 Value = -85.2°C, Uncertainty = 2.87°C,
Probability of Belonging to Distribution A = 0.67

Figure 82: Output from Validation Performed on Dataset with Random Heterogeneity (From Bimodal Heterogeneity Analysis)

Bimodal Heterogeneity - Maximum Likelihood Model

Combined Dataset - T0 Estimate = -60.8°C, Uncertainty = 4.39°C

Figure 83: Output from Validation Performed on Dataset with Random Heterogeneity (From Bimodal Heterogeneity Analysis – Combined Dataset)
Random Heterogeneity - Maximum Likelihood Model
Mean T0 Value = -62°C, Standard Deviation = 18°C

Figure 84: Output from Validation Performed on Dataset with Random Heterogeneity (From Random Heterogeneity Analysis)

Difference between Expected T0 Values for Individual Tests and Derived Mean T0 Value for Whole Dataset (-62°C), Sample of the Population - based upon Random Heterogeneity (Maximum Likelihood Model)

Figure 85: Output from Validation Performed on Dataset with Random Heterogeneity (From Random Heterogeneity Analysis) – Histogram
Figure 86: POR Test Specimens (Compact Tension Specimens with Semi-Elliptical Surface Defects) Analysed by Keim [153]
Figure 87: Master Curve Analysis of POR Specimens Analysed by Keim [153]

Figure 88: Master Curve Analysis of Standard Specimens Analysed by Keim [153]
Figure 89: Comparison of Constraint-Modified Fracture Toughness Curves (using different $m$ factors) [149] with Predictions of Fracture Toughness using Localised Effective Driving Force Model, $K_{MAT} = 50$ MPa√m

Figure 90: Comparison of Constraint-Modified Fracture Toughness Curves (using different $m$ factors) [149] with Predictions of Fracture Toughness using Localised Effective Driving Force Model, $K_{MAT} = 75$ MPa√m
Figure 91: Comparison of Constraint-Modified Fracture Toughness Curves (using different $m$ factors) [149] with Predictions of Fracture Toughness using Localised Effective Driving Force Model, $K_{MAT} = 100 \text{ MPa} \sqrt{m}$
Figure 92: Sectioning of the EURO Fracture Toughness Dataset Material [154]
SINTAP Lower Tail Analysis (Stage 1)
T0 Value = -88.6°C, Uncertainty = 4.05°C, Potential heterogeneity

Figure 93 : Output from Validation Performed on EURO Dataset (From SINTAP Lower Tail Analysis – Stage 1)

SINTAP Lower Tail Analysis (Stage 2)
T0 Value = -78.2°C, Uncertainty = 4.05°C, Potential heterogeneity

Figure 94 : Output from Validation Performed on EURO Dataset (From SINTAP Lower Tail Analysis – Stage 2)
Bimodal Heterogeneity - Maximum Likelihood Model
Distribution A - T0 Value = -82.9°C, Uncertainty = 0.85°C,
Distribution B - T0 Value = -111.3°C, Uncertainty = 2.06°C,
Probability of Belonging to Distribution A = 0.91

Figure 95: Output from Validation Performed on EURO Dataset (From Bimodal Heterogeneity Analysis)

Bimodal Heterogeneity - Maximum Likelihood Model
Combined Dataset - T0 Estimate = -84.5°C, Uncertainty = 4.05°C

Figure 96: Output from Validation Performed on EURO Dataset (From Bimodal Heterogeneity Analysis – Combined Dataset)
Random Heterogeneity - Maximum Likelihood Model
Mean T0 Value = -85°C, Standard Deviation = 10°C

Figure 97: Output from Validation Performed on EURO Dataset (From Random Heterogeneity Analysis)
6. IN-PLANE CONSTRAINT EFFECT ON FRACTURE TOUGHNESS IN SEN(B) SPECIMENS

6.1 INTRODUCTION

The use of plane strain fracture toughness in R6 assessments is generally considered conservative, since it is conventionally derived from deeply cracked bend specimens using recommended testing standards and validity criteria [R6, Section III.7]. The criteria are designed to ensure plane strain conditions and high hydrostatic stresses near the crack tip. The loss of in-plane constraint, perhaps due to shallow cracks or small ligaments, can contribute to increased effective fracture toughness values.

Some nuclear plant components have thin sections, such as the tubes and sleeves of the fuel plug unit assemblies. It has been postulated that the effective fracture toughness of these components may be higher than that which would be used in a standard assessment, due to the loss of out-of-plane constraint associated with the small thickness, or the loss of in-plane constraint associated with small cracked ligaments. It was decided that the potential increase in effective fracture toughness due to the loss of in-plane constraint would be assessed through a series of fracture toughness tests, performed at EDF Energy [157]. These tests would look at the effect of in-plane constraint on apparent fracture toughness, in thin width (W) single edge notched four point bend (SEN(4PB)) specimens with small ligaments. Out-of-plane constraint loss affects the fracture toughness associated with through-wall defects that grow around the circumference of the component, and this will be considered later in the thesis.

A series of finite element analyses (FEA) have therefore been performed to assist with the analysis of these tests. The FEA was also designed to identify if recommendations could be made to enhance the R6 procedure with advice on fracture toughness testing of low constraint geometries, and to suggest adjustments to well-documented fracture toughness data to make them more appropriate for defect tolerance assessment of low constraint geometries.

This work does not assess the influence of constraint on the material resistance to fracture, which depends upon the material constants $\alpha$ and $k$ (R6, Section III.7.5.3, developed from the work of Ainsworth [158]), but rather focuses the influence of the effects of structural constraint on the crack driving force, characterised by $\beta$, and the ability of a thin-width bend specimen to characterise
fracture toughness. In order to predict the constraint sensitivity of a specific material and the actual increase in fracture toughness of the material, it would be necessary to perform more detailed FEA with failure models, or undertake a test programme, and this could be performed in further work, as discussed later.

6.2 BACKGROUND

6.2.1 Testing

Figure 98 presents the test specimen geometry: a SEN(4PB) specimen. This was selected over the standard three-point bend test specimen, since the cracked ligaments are very small for a thin-width specimen and it was felt undesirable to apply the loading from the roller directly through the cracked ligament, however the cracked ligament is still under pure bending.

Fracture toughness properties may be derived from the specimen tests, through calculation of the $J$ integral from a load-displacement curve of a specimen, as described earlier in Section 2.3.4.1. It should be made clear that the SEN(4PB) specimen is not a standard specimen and the standard [32] does not provide advice on how such a specimen should be tested, or how the test data should be analysed. However, it is considered that the method of calculation of the $J$ integral from a load-displacement curve for this specimen should be comparable to that for more standard specimens. It should be noted that for significant loss of constraint, the validity of the $J$ integral as a parameter for uniquely characterising the fracture behaviour of a component is diminished. More discussion regarding the appropriateness of the method is given throughout the presentation of the results of this analysis.

The $J$ integral, as described in Section 2.3.4 (Equation 19) can be written as a function of $\eta_p$, which may be derived for a particular geometry using FE modelling, given that the $J$ integral may be derived with elastic-plastic finite element analyses.

6.2.2 Constraint

The $J$ integral becomes invalid as a crack tip parameter which can uniquely characterise the fracture behaviour of a component, when the large strain region reaches a finite size relative to in-plane dimensions. In this instance, two-parameter fracture mechanics can be used.

R6 Section III.7 currently only takes account of in-plane constraint in a particular specimen geometry under plane strain conditions. This is done using a normalised parameter, $\beta$, defined in terms of the constraint parameters $T$ (elastic) and $Q$ (elastic-plastic), using the relationships of
Equation 95. R6 Section IV.5 contains a compendium of $\beta$ solutions for various geometries, although only $\beta_T$ solutions are currently included. The $\beta_T$ solutions listed in R6 Section IV.5 are based upon limit load solutions assuming plane strain conditions.

For values of $\beta_T$ greater than zero (signifying high in-plane constraint), there is considered to be no benefit to the inclusion of constraint effects in the assessment of defect tolerance, and the standard procedure of R6 is therefore used.

A $\beta_T$ solution for a single edge cracked plate under bending (for a half span to width ($H/W$) ratio of 6) is provided in R6 Section IV.5.4.5. A polynomial was fitted to the data and is shown in Figure 99. Note for $a/W > 0.35$, $\beta_T > 0$ (i.e. exhibits high constraint).

6.2.3 Crack Tip Modelling

As discussed in Section 5.3.2, sharp cracks are usually modelled in a FE model using small-strain assumptions. Focused meshes should normally be used for small-strain fracture mechanics evaluations. For a sharp crack the strain field becomes singular at the crack tip. Generally, the mesh design should take account of the singularity at the crack tip in small-strain analysis in Abaqus [151] through the choice of crack tip element type and mesh refinement. Including the singularity often improves the accuracy of the $J$ integral, because the calculated stresses and strains in the region close to the crack tip more closely follow the HRR solution under high constraint conditions.

The size of the crack-tip elements also influences the accuracy of the solutions; the smaller the radial and angular dimensions of the elements at the crack tip, the more accurate the stress and strain results will be and, therefore, the more accurate the contour integral calculations will be. Abaqus [151] suggests that in many cases, if sufficiently fine meshes are used, accurate contour integral values can be obtained without using singular elements.

The crack-tip strain singularity depends on the material model used. Linear elastic, perfectly plastic, and power-law hardening material models are commonly used in FEA for fracture mechanics models. In Abaqus the Ramberg-Osgood deformation plasticity model, with von Mises yielding behaviour, is available, as described by Equation 13.

The Abaqus FE code does not model a pure linear elastic region when the deformation plasticity model is used i.e. the material behaviour described by the model in Abaqus is nonlinear at all stress levels, but for commonly used values of the hardening exponent ($n \sim 5$ or more), the nonlinearity only becomes significant for stresses approaching or exceeding $\sigma_0$ [151].
6.2.4  Tensile Testing

A number of tensile tests were carried out, by EDF Energy [159], on unaged AISI Type 321 stainless steel plate at room temperature (22°C). Type 321 steel is similar to the standard 18/8 steel (Grade 304), but stabilised with titanium additions. The grade is often used because it is not sensitive to intergranular corrosion after heating at high temperatures (up to 800°C). Type 321 has good forming and welding characteristics, and good fracture toughness properties, even down to cryogenic temperatures. It typically has a 0.2% proof strength of 205 MPa and a tensile strength of 515 MPa [160]. Room temperature initiation fracture toughness values are typically of the order of 200 MPa√m [161].

The typical chemical composition of Type 321 is as shown in Table 9 (in wt%) [161]. The material tested is considered to be representative of the material used to construct some of the thin components where the results of this work could be useful.

The tensile tests were performed using an Instron testing machine, with the tensile testing method based on BS EN ISO 6891-1 and 6892-2 [162, 163]. Three tests were carried out using a dual averaging extensometer with two LVDTs, and displacement was calculated using the average of the two transducers. The test specimens were all flat tensile specimens, with a rectangular cross section. The nominal dimensions were a thickness of 2.87 mm, a width of 6 mm and a gauge length of 24 mm.

Three detailed stress-strain curves were produced as a result of this tensile testing and are shown in Figure 100. These curves have slight variations in stress-strain behaviour at small strains (i.e. up to 0.5%), but have similar 0.2% proof stresses and post yielding behaviour, and so are all considered to be representative of the material. A summary of all tensile data for unaged plate collected at 22°C is provided in Table 10. The 0.2% proof strengths were found to be in the range of 245-300 MPa and tensile strengths were found to be in the range of 592-626 MPa. The strength of the Type 321 specimens tested is therefore slightly greater than the typical values for this material.

Care should be taken that any approximation to the stress-strain data, for use in finite element modelling and fracture assessment, is a good fit to the tensile data at relevant strain levels of interest (R6, Section II.1.6). When global parameters are of interest (as they are in this analysis), such as the load versus J integral response, the tensile data should be fitted at lower strain levels. When local parameters, such as stresses and strains local to the crack tip are of interest, the tensile data should be fitted at higher strain levels.
At small strains, the material can be characterised by an exponent of approximately $n = 20$, as shown in Figure 101. At large strains, a smaller exponent would be appropriate. R6, Section II.1.6 suggests that for fits to large strains, a value of $n$ may be estimated using the following equation:

$$\frac{1}{n} = 0.3 \left( 1 - \frac{\sigma_y}{\sigma_u} \right)$$  \hspace{1cm} (104)$$

where $\sigma_y$ is the 0.2% proof stress obtained in a uniaxial tensile test and $\sigma_u$ is the ultimate tensile stress obtained from the engineering stress-strain curve of a uniaxial tensile test. Use of Equation 104 leads to an estimate for a value of $n$ of approximately 5.5 to 6.8 for a Ramberg-Osgood fit to large strains.

Three separate Ramberg-Osgood equations have therefore been used in the subsequent FE analyses to describe the stress-strain behaviour, with exponents of $n = 5$, 10 and 20, which are judged to bound the possible fits of interest. These fits are shown in Figure 101 for comparison with the tensile test stress-strain data.

It should be noted that Ramberg-Osgood fits with larger $n$ values approximate the stress-strain data at small strains much better (shown in Figure 102) than the fits with smaller $n$ values, which are more appropriate for characterising the stress-strain behaviour at larger strains. However, for the purposes of the generalised analyses, the three Ramberg-Osgood curves chosen allow an appreciation of the sensitivity of the material model in the fracture behaviour. The Ramberg-Osgood parameters used in the analyses are summarised in Table 11.

### 6.3 MODELLING APPROACH

#### 6.3.1 Overview

An assessment of the level of constraint and load-displacement behaviour in the test specimens was undertaken using 3D FEA. The modelling and analysis was undertaken using Abaqus Version 6.9-2.

This indicative analysis was performed in anticipation of test data which will support the hypothesis of increased effective fracture toughness with reduced in-plane constraint, and to identify if thin-width bend specimens are suitable for fracture toughness testing.
6.3.2  Geometry

The SEN(4PB) test specimen that was modelled is shown in Figure 98. The specimens were modelled in three-dimensions, to capture through-thickness variations of fracture mechanics parameters and stress fields.

A range of specimen widths were modelled \((W = 25 \text{ mm}, 10 \text{ mm}, 5 \text{ mm}, 4 \text{ mm}, 3 \text{ mm}, 2 \text{ mm})\), to allow the study of both a standard bend specimen \((W = 25 \text{ mm})\) and thinner width specimens. The width range of 2-5 mm is considered of interest due to potential correlation with the thin components in plant. The specimen thickness \((B = 25 \text{ mm})\) was kept constant for all meshes. It should be noted that the locations of the test rollers, and hence the span, are dependent upon the width of the specimen, through the relationship:

\[
L = 2L_1 = 8W
\]

where \(L\) is the distance between the loaded rollers, and \(L_1\) is the distance between a fixed and loaded roller.

A series of quarter-model meshes were constructed using planar symmetry about the crack face plane and at the mid-plane in the out-of-plane direction. Each specimen width was modelled with four different crack depths \((a/W = 0.2, 0.4, 0.6, 0.8)\). A summary of the dimensions of the various models is summarised in Table 12.

20-noded quadratic elements with reduced integration were used in the linear elastic analyses (Abaqus element type C3D20R). 8-noded elements with reduced integration were used in the elastic-plastic analyses (Abaqus element type C3D8R) to reduce computational cost. A scoping study was carried out on one of the standard width geometries \((W = 25 \text{ mm})\) and it was shown that the differences in crack tip parameters (extracted at the contour integrals sufficiently far away from the crack tip), between 8-noded and 20-noded element meshes, were small. Contour values (e.g. for the \(J\) integral) at the crack tip were different. However, improved accuracy of modelling of the fracture mechanics parameters at the crack tip was not essential for this analysis, since the global stress fields and displacements were of more importance. It was found that the global stress field and the global displacements were almost identical for small strains. The use of 8-noded elements was therefore considered adequate for the purposes of the elastic-plastic analyses, to save on computational effort.

In order to minimise modelling uncertainty, a highly refined and focused mesh was employed at the crack tip location with 8 angular elements around the semi-plane. Elements were spaced so that the distance between the contour integrals became geometrically smaller (with a fixed scaling
factor on element width of 1.18) towards the crack tip elements (which had a length of $1 \times 10^{-2}$ mm). At the crack tip, collapsed elements were used, with coincident nodes at the crack tip merged to a single node for elastic analyses, and coincident nodes permitted to move independently for elastic-plastic analyses. In the elastic analyses, the mid-side nodes of the crack tip elements, along the edges which extend radially from the crack tip, were moved to the quarter-points (25% of the distance from the crack tip). This ensures an $r^{-1/2}$ crack tip singularity which is appropriate for linear elastic fracture mechanics. For the elastic-plastic analysis, linear elements without mid-side nodes were used.

Figure 103 shows two of the meshes used in the analyses, with Figure 104 showing a close up of one of the crack tip area meshes.

### 6.3.3 Material Properties

Values of Young’s modulus and Poisson’s ratio were chosen based on the parameters in Table 11, which are considered to be appropriate for stainless steels close to ambient temperature.

A nominal yield stress (i.e. 0.2% proof stress) value of 300 MPa was chosen for the elastic-plastic material model, as it is similar to values of 0.2% proof stress obtained from the testing of Type 321 stainless steels discussed in Section 6.2.4. The Ramberg-Osgood nonlinear elastic-plastic material model (Equation 13, as described in Section 6.2.3) was used to define the stress-strain curve in these analyses. Parameters used in the model are summarised in Table 11. Three different hardening exponents were assumed ($n = 5, 10, 20$). These exponents were selected to cover a range of values that might be expected for the materials of interest. As discussed in Section 6.2.4, the material of interest for this study can be characterised for small strains by an exponent of approximately $n = 20$. The sensitivity of the results to the values of the yield stress was not investigated.

### 6.3.4 Loads and Boundary Conditions

For the linear elastic analyses, a concentrated nodal force of 200 N was applied to a reference point, kinematically constrained to all nodes in the model representing the loading rollers. A nodal force of 200 N distributed across each roller location led to an applied bending moment ($M$) at the crack plane of varying magnitude depending on the specimen geometry (equal to $M = FL$, see Table 12).

For the elastic-plastic analyses, the magnitude of the applied load ($M$) was uniquely defined for each particular geometry, depending on the calculated limit load ($M_L$) for the geometry (R6, Section IV.5.4.5, using a plane strain von Mises formulation):
\[ M_L = \frac{\sigma_y BW^2}{2\sqrt{3}} \left(1 + 1.686a/W - 2.72(a/W)^2\right) \left(1 - a/W\right)^2 \quad \text{for} \quad a/W \leq 0.295 \tag{106} \]

\[ M_L = \frac{\sigma_y BW^2}{2\sqrt{3}} 1.2606(1 - a/W)^2 \quad \text{for} \quad a/W > 0.295 \tag{107} \]

The applied loadings were defined to cover an approximate range of \(0 < L_r < 2\). This range was reduced for the analyses using a hardening exponent of \(n = 20\). This range of loading is adequate to allow appropriate load-displacement curves to be produced, with ten equal loading steps defined. All of the analyses were based on a small-strain assumption for simplicity and consistency.

The models were physically constrained using a symmetric boundary condition on the crack plane, along the uncracked ligament (preventing in-plane rotation and axial displacement), and also along the mid-plane of the geometry (perpendicular to the crack plane). Applied loads and boundary conditions are shown in Figure 105 (symmetric boundary conditions not shown for clarity).

The direction of the initiation of cracking in this case was assumed to be along the crack plane, since the geometry and loading is symmetrical. However, it is noted that in reality, the direction of crack growth locally may not be along the symmetry plane (due to microstructural considerations). Crack tip parameters (\(J\) integral and \(T\) stress) were therefore extracted along this Virtual Crack Extension (VCE) direction. The parameters were extracted along 20 contours extending radially out from the crack tip. It is noted that the first two contour integrals were considered to be inaccurate in providing appropriate fracture mechanics data and were therefore excluded. Careful consideration was given to the contour dependence of the crack tip parameters through the thickness of the specimen, to ensure that appropriate values were chosen, since gradients near the surfaces can be significant due to the lower constraint.

### 6.4 RESULTS

#### 6.4.1 Linear Elastic Modelling

Figure 106 and Figure 107 show the variation of \(J\) integral and \(T\) stress across the contour integrals (at the mid-plane), for the 3 mm wide (\(W\)) specimen and the different crack depths studied, illustrating the contour independence. The near crack-tip \(T\) stresses exhibit slightly greater path dependence compared to that observed for the \(J\) integral. This level of contour independence exists for the other specimen widths.
Figure 108 shows the variation of $J$ integral across the specimen thickness (at the third contour integral), for the 3 mm wide specimen and the different crack depths studied (200 N applied loading in each case), illustrating reasonable contour independence through the thickness except at the free surface. A similar positional independence exists for the other specimen widths modelled.

Figure 109 shows the variation of $T$ stress across the specimen thickness (at the fifth contour integral), for the 3 mm wide specimen and the different crack depths studied (200 N applied loading in each case). Both Figure 108 and Figure 109 show the effect of the free surfaces on the fracture mechanics parameters, and the importance of analysing contour integral values across the thickness as well as radially from the crack tip, when selecting appropriate contour values.

Figure 110 shows the variation of $J$ integral with crack depth for the different specimen widths. $J$ was calculated as an average of the through-thickness values (based upon the third contour integral), excluding the surface element contour values. Figure 110 also includes the expected results based upon the relevant SIF solution from R6 Section IV.3.6.4 at different crack depths (with plane strain conditions assumed for calculating the $J$ integral values). It is noted that the FE predicted values agree well with those provided in R6 (i.e. within 5%). Clearly, the applied stress increases as width decreases due to the applied load being fixed, and the trend in $J$ with $B/W$ is therefore expected.

Figure 111 shows the variation of $J$ integral with crack depth (the FE derived values, and the values based on R6 Section IV.3.6.4), normalised by the reference stress for a bend specimen (given in R6 Section IV.1.5.6, a plane strain solution with the von Mises formulation). All the normalised $J$ integral values are similar (and comparable to the R6 values), with the thinner widths deviating from the plane strain values, as expected.

The comparisons of the textbook and FE derived $J$ integral values give confidence in the FE mesh to calculate the $T$ stress parameter adequately. Figure 112 shows the variation of $T$ stress with crack depth (for a 200 N applied loading in each case). The value of $T$ stress was calculated at the mid-plane (based upon the fifth contour integral). Since applied stress increases as width decreases (due to the applied load being fixed), the trend in $T$ with $B/W$ is expected.

$T/\sigma$ values, where $\sigma = (6M)/(BW^2)$ and $M =$ applied moment, were published by Sherry et al. [56], based on work by finite element modelling by Sham [164], which used higher order weight functions. Figure 113 shows the variation of $T$ stress normalised by the applied bending stress, with crack depth, for comparison with the values as calculated by Sham [164]. The FE values calculated here are seen to be very comparable to those calculated by Sham. The calculated values are within 5% of the Sham values for thinner specimens, but the discrepancy increases with increased width (due to the transition to plane strain behaviour).
Figure 114 shows the variation of $\beta_T$ with crack depth, for different specimen widths, which was derived using the reference stress solution for a bend specimen (given in R6 Section IV.1.5.1, a plane strain solution with the von Mises formulation). It is noted that the analyses yield similar results to those used to derive the $\beta_T$ solution of R6 Section IV.5.4.5 (shown in Figure 99). Constraint values are similar across the range of widths analysed. Constraint is negative below an $a/W$ value of approximately 0.35 (using linear interpolation). Constraint values derived from the analyses are summarised in Table 12 along with the crack tip parameters.

One important point to acknowledge is that in reality, components fail by plastic collapse as well as fracture and it is important to consider both failure mechanisms in any fracture assessment. To illustrate the interaction between the two failure mechanisms for this geometry and setup, $K_r$ and $L_r$ parameters for each configuration were plotted on Failure Assessment Diagrams (FADs), based on an Option 1 Failure Assessment Curve (FAC). Figure 115 and Figure 116 show the FADs for a 25 mm wide and 3 mm wide specimen respectively. The $L_r$ was based upon a 0.2% proof stress of 300 MPa. The $L_r$ cut-off value was based on a tensile strength of 450 MPa. $K_r$ was based upon the elastic SIF for the geometry (from R6 Section IV.3.6.4) and an initiation fracture toughness of 100 MPa√m. These FADs (which are not constraint modified) demonstrate that failure is dominated by plastic collapse (at least using the material properties chosen), and this is increasingly the case as the width of the specimen reduces.

### 6.4.2 Elastic-Plastic Modelling

Figure 117 shows the variation of $J$ integral across the contour integrals, at the mid-plane and normalised by the value at the tenth contour integral (0.07 mm from the crack tip), for the 3 mm wide specimen and a sample of the load steps. Figure 117 illustrates the dependence on contour selection as loading increases. This is due to the increase in plastic deformation around the crack tip with a smaller proportion of the plastic zone contained within the initial contour integrals. A similar contour dependence exists for all the other specimen widths and ligament ratios. To be consistent, the tenth contour value is used in all analyses to derive the $J$ integral, noting that the contour dependence is significant for loadings larger than $L_r = 1.4$.

Figure 118 shows the variation of $J$ integral across the specimen thickness normalised by the mid-plane value for the 3 mm wide specimen and for a sample of the load steps. Figure 118 illustrates the positional-dependence through the thickness of the specimen. This dependence exists for all specimens and crack depths, at all load steps.

Table 13 summarises selected crack tip parameters (knife edge opening displacement and total $J$ integral) extracted from selected analyses ($W = 3$ mm, $n = 10$). The $J$ integral is an average of
the through-thickness values (based upon the tenth contour integral), excluding the surface element contour values, and the displacement was based upon the knife edge opening displacement at the mid-plane.

Load-displacement curves were derived for each configuration. Sample load-displacement curves are shown in Figure 119 for the 25 mm width specimen \( (n = 10) \), at various crack depths.

The results of the elastic-plastic modelling can be used to calculate \( \eta_p \) values as discussed in Section 2.3.4.1. Equation 19 may be rearranged to give an estimate for \( \eta_p \):

\[
\eta_p = \left( \frac{J_p}{b\sigma_y} \right) \div \left( \frac{U_p}{b^2 B\sigma_y} \right)
\]

\( \eta_p \) can therefore be found easily through linear regression of Equation 108. Figure 120 shows an example of the \( \eta_p \) values calculated for the 25 mm width specimen \( (n = 10) \), with the varying crack depths. \( J_p \) was calculated by subtracting the elastic \( J_e \) (calculated from R6 Section IV.3.6.4, assuming plane strain conditions) from an average of the through-thickness values of Abaqus calculated values of \( J \) (based upon the tenth contour integral), excluding the surface element contour values. \( U_p \) was based upon the displacement at the mid-plane. It is noted that if \( U_p \) was based instead upon an average displacement across the thickness, then the \( \eta_p \) values obtained would be slightly different (and only significantly different for specimens with \( a/W = 0.2 \), where the displacement varies significantly through-thickness).

Figure 121, Figure 122 and Figure 123 show variations of \( \eta_p \) values versus \( a/W \), for different width specimens for hardening exponents \( n = 5, 10 \) and 20 respectively. There is significantly more variation in \( \eta_p \) values for different bend specimen widths at an \( a/W \) of 0.2, than for the more deeply cracked specimens. This variation is likely due to the different plastic strains in the ligament for any given loading. Further analysis would be required to identify the exact effect of the material hardening exponent on the relationship.

Kim [165] proposed the following solution for \( \eta_p \) for SEN(4PB) specimens using 2D plane-strain FE analyses, based on crack mouth opening displacement (which is comparable to the knife edge opening displacement):

\[
\eta_{p,CMOD} = \left[ \frac{(L + 2L_1) - L}{4W} \right]^{4.0 - 2.08 \left( \frac{a}{W} \right)}
\]

For the geometry analysed in this study, \( L_1 = 4W \). This solution can be simplified as:
Since this linear equation does not include any dependence on the hardening exponent or explicit dependence upon width, it yields different $\eta_p$ values than those predicted in the current analyses, although it is broadly consistent with the general trend. Equation 110 is plotted in Figure 121, Figure 122 and Figure 123 for comparison with the $\eta_p$ values derived in the current analyses.

These $\eta_p$ values should be used in fracture mechanics testing of SEN(4PB) specimens to derive $J$ integral values at fracture and hence effective fracture toughness values for a given configuration.

### 6.4.3 Modified Boundary Layer

A modified boundary layer (MBL) model was used to investigate the relationship between the specimen width and the elastic-plastic crack tip constraint. The MBL model was set up as a semi-circle with a large radius ($r = 1000$ mm) to ensure small scale yielding (SSY). Only one half of the MBL model was required due to symmetrical loading in the specimen models.

Boundary conditions were applied at the surface controlled by the elastic $K$-field and $T$ stress. The load was applied through the boundary conditions using a displacement field $(u, v)$ controlled by the elastic asymptotic stress field of a plane strain Mode-I crack, based on work by Larsson and Carlsson [50]:

\[
\begin{align*}
u(r, \theta) &= K_I \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \sin \left( \frac{1}{2} \theta \right) \left( 3 - 4v - \cos \theta \right) - T \frac{1 - \nu^2}{E} r \cos \theta \\
u(r, \theta) &= K_I \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \cos \left( \frac{1}{2} \theta \right) \left( 3 - 4v - \cos \theta \right) + T \frac{1 - \nu^2}{E} r \sin \theta \end{align*}
\]

where $K_I = \sqrt{(EJ/(1-\nu^2))}$ under plane strain conditions; $r$ and $\theta$ are polar coordinates centred at the crack tip with $\theta = 0$ corresponding to the uncracked ligament ahead of the crack tip.

CPE8R 8-noded plane strain elements with reduced integration were used in the MBL model, with the size of elements decreasing geometrically as they approach the crack tip. The length of the crack tip elements was $0.01$ mm. Material properties used in the MBL model were the same as those used in the analysis of the specimen (see Table 11).
An MBL analysis was carried out for a range of applied loadings (different $J$ values) with zero $T$ stress, to obtain the SSY normalised opening stress curve for each material hardening exponent used in the main analyses. Figure 124 is a plot of the normalised opening stresses for a range of applied loadings, against the distance ahead of the crack tip, normalised by crack driving force, $r/(J/\sigma_y)$, for the SSY solution with a hardening exponent of $n = 10$. Figure 124 shows that the normalised opening stress fields collapse onto a single curve – the SSY curve. This is also true for the other hardening exponents analysed. The SSY curves were used as a reference curve for calculation of a $Q$ parameter.

MBL analyses were also carried out for a specific applied loading ($J = 100$ N/mm) with a range of $T$ stress values. Figure 125 shows that the normalised opening stress field exhibits a hydrostatic shift from the SSY stress field (a loading with a $T$ stress value of zero).

Opening stresses from a sample of the specimens analysed in the elastic-plastic modelling of Section 6.4.2, were extracted ahead of the crack tip, for each of the ten loading steps in each analysis:

- $W = 25$ mm, $a/W = 0.2$ and 0.6, $n = 10$
- $W = 5$ mm, $a/W = 0.2$ and 0.6, $n = 10$
- $W = 3$ mm, $a/W = 0.2$ and 0.6, $n = 10$
- $W = 3$ mm, $a/W = 0.2$ and 0.6, $n = 5$
- $W = 3$ mm, $a/W = 0.2$ and 0.6, $n = 20$

Figure 126 shows the opening stress field in an MBL model, where the displacement field applied was based upon the elastic-plastic $J$ integral and $T$ stress results from the elastic-plastic modelling of Section 6.4.2, for the specific case of $W = 3$ mm, $a/W = 0.2$, $n = 10$, and $M = 18000$ Nmm, noting that Equations 111 and 112 are plane strain formulations. Compared to the significant plasticity in the actual specimen for this particular loading configuration, the plasticity is contained in the MBL model.

The opening stress fields from the bend specimen analyses specified above, were normalised and plotted against the normalised distance parameter $r/(J/\sigma_y)$. A sample of one of these plots for one of the loading configurations ($W = 3$ mm, $a/W = 0.2$, $n = 10$) is presented in Figure 127. This figure illustrates how the normalised stresses can deviate away from the SSY stresses as loading increases, with the $J$ integral converted to the non-dimensional loading parameter $J/(a\sigma_y)$. There is
increased deviation from the SSY curve in thinner specimens, for similar normalised $J$ loadings. This occurs due to the increased interaction of the compressive stresses (at the free surface) with the tensile stresses (at the crack tip), leading to a reduced normalised stress at a given normalised load.

The $Q$ parameter is calculated based upon the difference between the SSY normalised opening stress and the normalised opening stress (see Equation 28). $Q$ parameters were only derived for load steps which did not invalidate the assumptions of the equation. Load steps with high $J$ integral values were excluded, since the $r = 2J/\sigma_y$ value would be greater than the length of the ligament. Load steps with low $J$ values were excluded, since the $r = 2J/\sigma_y$ value would be smaller than the radial position of the second contour integral and therefore invalid.

The derived $Q$ parameters are plotted against the normalised $T$ stress in Figure 128. A bi-linear fit to the data is also shown, in comparison to the bi-linear equation of R6 Equation III.7.4, developed from Ainsworth and O’Dowd [147] for primary loading:

$$Q^p = T^p / \sigma_y \quad \text{for } -0.5 < T^p / \sigma_y \leq 0$$
$$Q^p = 0.5T^p / \sigma_y \quad \text{for } 0 < T^p / \sigma_y \leq 0.5$$

It is acknowledged that R6 Equation III.7.4 is relevant for configurations where $L_r \leq 0.5$ and many of the $Q$ parameters plotted are derived from analyses which do not satisfy that condition (this would explain the deviation of the FE derived values from Equation 113). For a given configuration and hardening exponent, an increase in load leads to an increase or a decrease in the $T$ stress (and a corresponding change in the $Q$ parameter), depending on whether the configuration is a low or high constraint geometry (i.e. whether $T$ stress is less than or greater than zero). The trend appears to follow common understanding, with negative normalised $T$ stresses generally corresponding to negative $Q$ parameters, and vice versa. The $Q$ versus $T$ stress relationship does appear to have some dependency upon the width of the specimen and the hardening exponent.

$J$ integral values are plotted against the $Q$ parameters in Figure 129 (for the low constraint specimens i.e. $a/W = 0.2$), to establish $J$-$Q$ loci which may be helpful in determining effective fracture toughness during testing of thin width bend specimens. There is a general trend of an increase in $J$ integral value with decreasing $Q$ parameter, with variance depending on the specimen width and hardening exponent. It should be noted that some of the $J$-$Q$ locus points plotted are not necessarily relevant to a constraint condition at a critical criterion of fracture.
It is also worth noting that the $Q$ parameters which are presented in the above figures were calculated at loadings associated with small amounts of plasticity. However, a modified $Q$ parameter was suggested by Zhu and Leis [166] amongst others, to account for bending-dominant large deformation. The approach has not been analysed in detail, although further work could investigate the effect of this calculation method on the derivation of $Q$, if a more thorough analysis of the $J$-$Q$ relationships at larger deformations were required.

6.5 DISCUSSION

6.5.1 Comparison with Data from the Literature

Hadley and Karger [167] assessed the effect of crack tip constraint in standard size (50 mm thick, 25 mm width) bend specimens (A533B steel at -100$^\circ$C), as part of the validation of the methods included in SINTAP for dealing with crack tip constraint. Figure 130 shows the results of this analysis, showing that for low constraint conditions, the apparent fracture toughness increases significantly above the plane strain fracture toughness.

Rathbun et al. [168] assessed in-plane constraint loss for a typical low alloy pressure vessel steel in the DBT transition region, to identify increases in apparent fracture toughness. A database of fracture toughness values was developed for a homogenous plate section of the decommissioned Shoreham Reactor vessel steel (ASTM A533B) on bend specimens with a range of thicknesses $B$ ranging from 7.9 mm to 254 mm, and width $W$ ranging from 6.4 mm to 508 mm. Some of this data have been manipulated and shown in Figure 131. There is seen to be some effect of specimen width (for a given specimen thickness) on the level of constraint (and the subsequent apparent fracture toughness measurement).

Both these studies were more relevant for assessing the effect of crack tip constraint on brittle fracture (ferritic steel at cool temperatures), although there is comparability between the geometric constraint parameters calculated here and as part of the thesis, and a demonstration of the subsequent effect on apparent fracture toughness. Hadley and Karger [167] noted that some of the increase in apparent fracture toughness may have been due to an increased amount of ductile tearing prior to fracture. Generally, the thin width bend specimen is considered to be adequate as a specimen type for assessing the effect of in-plane constraint, although it is more acceptable for material types with high strengths such as the A533B steels studied by Hadley and Karger [167] and Rathbun et al. [168].
6.5.2 Technical Outcomes

The modelling carried out during this study has allowed the following improvements in technical understanding:

- An appreciation of the variance in elastic and elastic-plastic in-plane geometric constraint in varying widths of bend specimens.

- More detailed definitions of plastic eta factor, and their dependence on width, crack depth, and material hardening exponent, than provided in the literature. These relationships should be used to assist with the analysis of thin width bend specimens.

- A relationship between elastic and elastic-plastic in-plane constraint was constructed, which appears to agree well with common understanding for small deformations, however the deviation from common understanding during large deformation, for different specimen widths and material hardening exponents is of interest.

- \( J-Q \) loci were created which will be of use in understanding correlations between \( J \) and \( Q \) during testing of different width specimens.

- Testing of thin width bend specimens will allow characterisation of increased apparent fracture toughness, if tensile properties are sufficient to prevent plastic collapse.

6.6 CONCLUSIONS

Fracture mechanics parameters (\( J \) integral, elastic \( T \) stress, elastic-plastic in-plane constraint parameter \( Q \)) were derived for SEN(4PB) specimens under various loading configurations using finite element analysis. This work was undertaken to assess the effect of in-plane constraint on fracture toughness. This work does not assess the influence of constraint on the material resistance to fracture, but rather focuses on the influence of the effects of structural constraint on the crack driving force, characterised by \( \beta \), and the ability of a thin-width bend specimen to characterise fracture toughness. In order to predict the constraint sensitivity of a specific material and the actual increase in fracture toughness of the material, it would be necessary to perform more detailed FEA with failure models, or undertake a test programme.

The \( \beta_T \) elastic in-plane structural constraint factor was derived for different specimen widths of SEN(4PB) specimens, and the analysis showed that different width specimens generally have comparable elastic in-plane constraint.
Plastic eta ($\eta_p$) factors were derived for different widths of specimen, and the dependence upon $a/W$ and material hardening was analysed. These $\eta_p$ factors may be used to derive critical $J$ integral values during fracture toughness testing of thin width specimens. $\eta_p$ factors are most dependent on specimen width at small $a/W$ values (where in-plane constraint loss is significant).

The elastic-plastic in-plane structural constraint factor $Q$ was derived for different specimen widths of SEN(4PB) specimens, and the analysis showed that thinner width specimens have reduced elastic-plastic in-plane constraint. $J-Q$ loci were created which will be of use in understanding correlations between $J$ and $Q$ during testing of different width specimens. The trends inferred from the relationship between elastic $T$ stress and the $Q$ parameter for these geometries are consistent with those in the literature, but there are deviations dependent on the specimen width and the material hardening exponent. Further analysis is needed to derive robust relationships between these assessment parameters.

It should be noted that the SEN(4PB) specimen design modelled in this study is intended for situations where the loss of in-plane constraint is considered to be important for accurate estimation of fracture toughness. Out-of-plane constraint effects are not considered in this study. The reason for studying this geometry was to ensure low constraint conditions, and to allow an appreciation of the effects of loss of geometric constraint in thin-width geometries. Testing of thin width bend specimens will allow characterisation of increased apparent fracture toughness.

However, it should be noted that two-parameter approaches to fracture mechanics are known to break down under large scale yielding conditions, and three-parameter approaches may also have reduced validity in these circumstances. Prediction of increased apparent fracture toughness is only useful for specimens with sufficiently high tensile properties, otherwise plastic collapse is more likely to be the dominant failure mode. It is important to consider each potential failure mechanism in any fracture assessment.

### 6.7 SUGGESTED FUTURE WORK

The modelling contained in this study may support ongoing fracture mechanics tests of SEN(4PB) specimens at EDF Energy. There is an indication that thin width SEN(4PB) specimens will have a higher effective fracture toughness than the thicker width specimens.

However, this study does not assess the influence of constraint on the material resistance to fracture, but rather focuses on the influences of the effects of structural constraint on the effective crack driving force, and the capability of thin width bend specimens to provide accurate fracture toughness values. In order to predict the constraint sensitivity of the material and the actual
increase in fracture toughness of the material, it would be necessary to perform more detailed FEA
with failure models in the material definitions, or undertake a test programme. Further analysis
may be desirable to provide estimates of increased effective fracture toughness in thin width bend
specimens.

Further analysis may also be desirable, and could provide improved estimates of elastic-plastic
in-plane constraint, if bending-dominant large deformation was taken into account. Future work
could also investigate constraint behaviour in thin section specimens with significant welding
residual stresses and subsequently include analysis of the effects of weld mismatch and residual
stresses on crack tip constraint.
Table 9: Chemical Composition of Type 321 Stainless Steel Plate (in wt%) [161]

<table>
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<tr>
<th>C</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mn</th>
<th>Ni</th>
<th>N</th>
<th>Ti</th>
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Table 10: Tensile Testing of Type 321 Plate [159]

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<th>UTS (GPa), $\sigma_u$</th>
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</thead>
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<tr>
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<td>592</td>
</tr>
<tr>
<td>5488-9-1-3 (3 mm plate) LT</td>
<td>258</td>
<td>592</td>
</tr>
<tr>
<td>5488-10-14 to 19 (3 mm plate) LT</td>
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<td>625</td>
</tr>
<tr>
<td>5488-9-3-2-17 (3 mm plate) LT</td>
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<td>625</td>
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<td>5488-9-3-2-18 (3 mm plate) LT</td>
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<td>625</td>
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<td>5488-10-13 (19 mm plate) LT</td>
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<td>625</td>
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<tr>
<td>5488-9-3-2-1 to 5 (3 mm plate)* TL</td>
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<td>622</td>
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Note – (*) specimens cut to 3 mm thick from 19 mm thick rolled plate. Other specimens cut from 3 mm rolled plate. LT/TL = longitudinal/transverse, transverse/longitudinal direction.
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<td>Hardening Exponent, $n$</td>
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<td>Yield Offset, $\alpha$</td>
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Table 11: Ramberg-Osgood Parameters
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**Note** – $T$ Stress is based upon the third contour integral at the mid-plane. SIF is the through-thickness average of the third contour integrals, excluding the surface element contour integral values.

**Table 12**: Fracture Mechanics Parameters Extracted from Linear Elastic Analyses of SEN(4PB) Specimens (Applied Load of 400 N)
<table>
<thead>
<tr>
<th>$a/W$</th>
<th>$J$ (N/mm)</th>
<th>CMOD (mm)</th>
<th>$a/W$</th>
<th>$J$ (N/mm)</th>
<th>CMOD (mm)</th>
<th>$a/W$</th>
<th>$J$ (N/mm)</th>
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**Note** – CMOD is based upon the displacement of the distance between the knife edges (at the mid-plane). $J$ is the through-thickness average of the tenth contour integrals, excluding the surface element contour integral values.

**Table 13 : Fracture Mechanics Parameters Extracted from a Sample of the Elastic-Plastic Analyses of SEN(4PB) Specimens ($W = 3$ mm, $n = 10$)**
Figure 98: Suggested SEN(4PB) Test Geometry

Specimen

Loaded Rollers

Fixed Roller

Fixed Roller

Clip gauge attachment knife edges

Specimen

L_1 = 4W
L = 8W

L_1 = 4W

W

6 mm

6 mm

10 mm

60°

>5 mm

B
Figure 99: $\beta_T$ vs. $a/W$ – Single Edge Cracked Plate under Bending ($H/W = 6$), R6 [4]

Section IV.5.4.5
Figure 100: Experimental Tensile Data [159]

Figure 101: Experimental Tensile Data [159] and Ramberg-Osgood Curves Used in the Analyses (Fits at Small Strains)
Figure 102: Experimental Tensile Data [159] and Ramberg-Osgood Curves Used in the Analyses (Fits at Large Strains)

Figure 103: Sample of the SEN(4PB) Meshes Used in the FE Analyses (Quarter Symmetry Models), a) $W = 3 \text{ mm, } a/W = 0.4$, b) $W = 25 \text{ mm, } a/W = 0.4$
Figure 104: Sample of the SEN(4PB) Meshes Used in the FE Analyses – Crack Tip Close-Up

Figure 105: Boundary Conditions in the FE Analyses (Symmetric Boundary Conditions Not Shown), a) $W = 3$ mm, b) $W = 25$ mm
Figure 106: 3D FE Analysis ($W = 3\text{ mm}$) – Linear Elastic – $J$ Integral (At Mid-Plane) vs. Contour Number, Applied Loading = 200 N

Figure 107: 3D FE Analysis ($W = 3\text{ mm}$) – Linear Elastic – $T$ Stress (At Mid-Plane) vs. Contour Number, Applied Loading = 200 N
Figure 108: 3D FE Analysis ($W = 3$ mm) – Linear Elastic – $J$ Integral (Based Upon Third Contour Integral) vs. Distance Along Crack Front ($z/B = 0$ at Surface), Applied Loading = 200 N

Figure 109: 3D FE Analysis ($W = 3$ mm) – Linear Elastic – $T$ Stress (Based Upon Third Contour Integral) vs. Distance Along Crack Front ($z/B = 0$ at Surface), Applied Loading = 200 N
Figure 110: SEN(4PB) $J$ Integral (Third Contour Integral Averaged Through-Thickness) vs. $a/W$ (Comparison with R6 Section IV.3.6.4) – Linear Elastic Analysis, Applied Loading = 200 N

Figure 111: SEN(4PB) $J$ Integral (Third Contour Integral Averaged Through-Thickness), Normalised by the Reference Stress, vs. $a/W$ (Comparison with R6 Section IV.3.6.4) – Linear Elastic Analysis
Figure 112: SEN(4PB) $T$ Stress (Fifth Contour Integral at Mid-Plane) vs. $a/W$ – Linear Elastic Analysis, Applied Loading = 200N

Figure 113: $T$ Stress (Fifth Contour Integral At Mid-Plane) Normalised by Uncracked Applied Stress versus $a/W$ – Comparison with Sham [164] Analysis
Figure 114: SEN(4PB) $\beta_r$ vs. $a/W$ (Evaluated at Mid-Plane)

Figure 115: Failure Assessment Diagram – SEN(4PB), $W = 25$ mm
Figure 116: Failure Assessment Diagram – SEN(4PB), $W = 3$ mm

Figure 117: $W = 3$ mm, $a/W = 0.6$ – Elastic-Plastic Analysis – $J$ Integral (At Mid-Plane) versus Contour Number, Normalised by the Tenth Contour Value, for a Sample of Load Steps, $n = 10$
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Figure 130: Increase in Apparent Fracture Toughness with Reduction of Constraint in A533B Steel [167]
Figure 131: Variation in Apparent Fracture Toughness with Specimen Width for Charpy Specimens [168]
7. OUT-OF-PLANE CONSTRAINT EFFECT ON FRACTURE TOUGHNESS IN C(T) SPECIMENS

7.1 INTRODUCTION

As discussed previously, the use of plane strain fracture toughness in defect tolerance assessments (such as in the R6 procedure) is generally considered conservative, since it is conventionally derived from deeply cracked bend specimens using recommended testing standards and validity criteria [R6, Section III.7]. These criteria are designed to ensure plane strain conditions and high hydrostatic stresses near the crack tip. The loss of out-of-plane constraint, inherent in thin section components, can contribute to increased effective fracture toughness values.

It was decided that the potential increase in effective fracture toughness due to the loss of out-of-plane constraint would be assessed through a series of fracture toughness tests, performed at EDF Energy [157]. These tests would look at the effect of out-of-plane constraint loss on apparent fracture toughness, on small thickness ($B$) compact tension (C(T)) specimens.

A series of finite element analyses (FEA) have therefore been performed to assist with the analysis of these tests. The FEA was also designed to identify if recommendations could be made to enhance the R6 procedure with advice on fracture toughness testing of low constraint geometries, and to suggest adjustments to well-documented fracture toughness data to make them more appropriate for defect tolerance assessment of low constraint geometries.

This study provides a general indication of the influence of constraint on the material resistance to fracture through use of a ductility exhaustion damage model. However, increases in apparent fracture toughness due to loss of out-of-plane constraint are likely to be heavily material dependent and would require calibration of the damage model based upon experimental testing. It is worth noting that the proposed damage model is based upon the failure mechanism of the growth of a void reaching a critical size (leading to ductile fracture), and does not consider any other failure mechanisms (such as shear band localisation). An alternative damage model may be required under the circumstances of a different failure mechanism being dominant.
7.2 BACKGROUND

7.2.1 Testing

Figure 132 shows a straight notch C(T) specimen as recommended in the testing standards [32]. The thin section C(T) specimen that was tested by EDF Energy has been slightly modified over the standard 19 mm thickness specimen, by inclusion of a curved dove tail notch feature at the crack mouth, to facilitate placement of clip gauge knife edges. In the tests, anti-buckling plates were used to prevent out-of-plane movement.

As discussed previously, fracture toughness properties may be derived from the specimen tests, through calculation of the $J$ integral, using a load-displacement curve of a specimen, as described earlier in Section 2.3.4.1. It should be acknowledged that the thin C(T) specimen is not a standard specimen and the standard does not provide advice on how such a specimen should be tested, or how the test data should be analysed. However, it is considered that the method of calculation of the $J$ integral from a load-displacement curve for this specimen should be comparable to that for standard specimens. Section 6.2.1 provides a summary of the method used for deriving the $J$ integral from the tests.

It should be noted that for significant loss of constraint, the validity of the $J$ integral as a parameter for uniquely characterising the fracture behaviour of a component is diminished. More discussion regarding the appropriateness of the method is given throughout the presentation of the results of this analysis.

7.2.2 Constraint

As described in the previous studies, the $J$ integral becomes invalid as a crack tip parameter which can uniquely characterise the fracture behaviour of a component, when the large strain region reaches a finite size relative to the in-plane dimensions. In this instance, two-parameter fracture mechanics can be used.

R6 Section III.7 currently only takes account of in-plane constraint in a particular specimen geometry under plane strain conditions. This is done using a normalised parameter, $\beta$, defined in terms of the constraint parameters $T$ (elastic) and $Q$ (elastic-plastic), using the relationships of Equation 95. R6 Section IV.5 contains a compendium of $\beta$ solutions for various geometries, although only $\beta_T$ solutions are currently included. The $\beta_T$ solutions listed in R6 Section IV.5 are based upon limit load solutions assuming plane strain conditions. There are currently no methods for quantifying out-of-plane constraint in R6, as there are in R6 Section IV.5 for in-plane constraint.
R6 suggests instead that testing specimens with a thickness equal to the component thickness could be used to identify increases in apparent fracture toughness resulting from a reduction in out-of-plane constraint.

For values of $\beta_T$ greater than zero (signifying high in-plane constraint), there is considered to be no benefit to the inclusion of constraint effects in the assessment of defect tolerance, and the standard procedure of R6 is therefore used.

A $\beta_T$ solution for a C(T) specimen is not included in R6. However, $T/\sigma$ values (where $\sigma = P/(WB)$ and $P =$ applied load) were published by Sherry et al. [56], based on work by Leevers and Radon [52], which used a variation technique employing the principle of minimum energy for a two-dimensional plane strain geometry, and work by Kfouri [169], which used two-dimensional plane strain finite element analysis. A $\beta_T$ solution for use in the analysis of thin C(T) specimens would be desirable.

A triaxial stress constraint parameter that has been suggested by Guo [69] is the $T_Z$ parameter, as described by Equation 31. The $T_Z$ parameter is not an elastic parameter like the $T$-stress, but rather an elastic-plastic stress constraint parameter. For elastoplastic cracks, $T_Z$ varies between 0.5 and 0.0, corresponding to the limiting cases of plane strain and plane stress respectively. This parameter has therefore been investigated to identify if it can provide a reasonable description of the out-of-plane constraint loss, as well as a means of prediction of increased fracture toughness in thinner specimens.

### 7.2.3 Material Tests

#### 7.2.3.1 Tensile Testing

A number of tensile tests were carried out at room temperature on unaged 3 mm thick AISI Type 321 stainless steel plate, as discussed in Section 6.2.4. This material is considered to be representative of the material used to construct some of the thin components where this work could be useful in providing an enhanced understanding of the effect of out-of-plane constraint loss on apparent fracture toughness. Three stress-strain curves were produced, and these are shown in Figure 100. These curves have slight variations in stress-strain behaviour at small strains (i.e. up to 0.5%), but have similar 0.2% proof stresses and post yielding behaviour, and so are all considered to be representative of the material.
7.2.3.2 Fracture Toughness Testing

A number of fracture toughness tests were carried out, by EDF Energy [157], on C(T) specimens, constructed from nominally 3 mm thick AISI Type 321 stainless steel plates in the unaged and aged condition, and 3 mm thick specimens cut from unaged 19 mm thick C(T) specimens.

These tests were carried out at temperatures of 22°C, 500°C and 650°C in the longitudinal/transverse (LT) and transverse/longitudinal (TL) orientations using single specimen (unloading compliance) and multiple specimen (with unloading and without unloading compliance) techniques. The data was analysed by EDF Energy using in-house analysis software. The tests were carried out using a dual averaging extensometer with two LVDTs, and displacement was calculated using the average of the two transducers.

Initiation fracture toughness ($K_{0.2}$) values were derived from the data and are presented in Table 14. Specimens with the designation ‘5488-9-X’ were manufactured from rolled 3 mm plates in unaged and aged conditions. Specimens with the designation ‘5488-10-X’ were manufactured from unaged 25 mm rolled plate. The ‘5488-10-X’ plate was then subsequently machined into both 19 mm and 3 mm compact tension specimens to study the effect of thickness on fracture toughness. However, it was noted that there could be a through-thickness variation in the composition. Chemical analysis of the plate showed that the two specimen sets were sufficiently different such that tensile and fracture toughness properties are not directly comparable.

Figure 133 shows the variation of the fracture toughness data with temperature, for the three different fracture toughness data sets. The trends show that there is not any discernible distinction between the 3 mm and 19 mm thick specimens (if anything, the thicker specimens had a higher fracture toughness). However, there was also concern that a substantial amount of plasticity was observed to occur in many of the tests before fracture. This implies that the tensile properties may be too low to allow any enhancement in fracture toughness due to loss of constraint. Therefore, for the purposes of this study, indicative analysis was performed in anticipation of test data which will support the hypothesis of increased effective fracture toughness with reduced constraint.

7.3 MODELLING APPROACH

7.3.1 Overview

An assessment of the level of constraint and load-displacement behaviour in the thin C(T) test specimens was undertaken using 3D FEA. The modelling and analysis was undertaken using Abaqus Version 6.10-1.
This analysis was performed in anticipation of test data which will support the hypothesis of increased effective fracture toughness with reduced out-of-plane constraint.

### 7.3.2 Geometry

The C(T) test specimen modelled is shown in Figure 132. The specimen was modelled in three-dimensions, to capture through-thickness variations of fracture mechanics parameters and stress fields.

A range of specimen thicknesses were modelled ($B = 19$ mm, 10 mm, 5 mm, 4 mm, 3 mm, 2 mm), to allow the study of both the baseline thickness ($B = 19$ mm) and a range of thinner C(T) specimens. The thickness range of 2-5 mm is considered of interest due to potential correlation with thin components in nuclear plant. The specimen width ($W = 38$ mm) was kept constant for all meshes.

A series of quarter-model meshes were constructed, using planar symmetry about the crack face plane and at the mid-plane in the out-of-plane direction. Each specimen thickness was modelled with four different crack depths ($a/W = 0.4, 0.5, 0.6, 0.7$). A summary of the dimensions of the various models is summarised in Table 16.

20-noded quadratic elements with reduced integration were used in the linear elastic analyses (Abaqus element type C3D20R). 8-noded elements with reduced integration were used in the elastic-plastic analyses (Abaqus element type C3D8R) to reduce computational cost. A scoping study was carried out on one of the standard thickness geometries ($B = 19$ mm) and it was shown that the differences in crack tip parameters (extracted at the third contour integral away from the crack tip), between 8-noded and 20-noded element meshes, were very small. Contour values (e.g. for the $J$ integral) at the crack tip were different. However, improved accuracy of modelling of the fracture mechanics parameters at the crack tip was not essential for this analysis, since the global stress fields and displacements were of more importance. It was found that the global stress field and the global displacements were almost identical for small strains. The use of 8-noded elements was therefore considered adequate for the purposes of the elastic-plastic analyses.

Since stress gradients near the free surfaces of specimens can be significant, and this study is interested in monitoring the dependence of the stress state on the thickness, each modelled geometry had 20 elements through the half-thickness, and element widths through the thickness were chosen to be geometrically smaller as they approached the free surface (with a fixed scaling factor on element width of 1.15). The elements at the free surface had an approximate width of 0.5% of the thickness, and the elements at the mid-plane had a width of approximately 7% of the thickness.
In order to minimise modelling uncertainty, a highly refined and focused mesh was employed at the crack tip location with 8 angular elements around the semi-plane. Elements were spaced so that the distance between the contour integrals became geometrically smaller (with a fixed scaling factor on element width of 1.33) towards the crack tip elements (which had a length of $3 \times 10^{-4}$ mm). At the crack tip, collapsed elements were used, with coincident nodes at the crack tip merged to a single node for elastic analyses, and coincident nodes permitted to move independently for elastic-plastic analyses. In the elastic analysis, the mid-side nodes of the crack tip elements, along the edges which extend radially from the crack tip, were moved to the quarter-points (25% of the distance from the crack tip). This ensures an $r^{-1/2}$ crack tip singularity which is appropriate for linear elastic fracture mechanics. For the elastic-plastic analysis, elements without mid-side nodes were used. Figure 134 shows two of the meshes used in the analyses, with Figure 135 showing a close up of one of the crack tip area meshes.

### 7.3.3 Material Properties

Values of Young’s modulus and Poisson’s ratio were chosen to be appropriate for stainless steels close to ambient temperature. These parameters are summarised in Table 15.

A nominal yield stress (i.e. 0.2% proof stress) value of 300 MPa was chosen for the elastic-plastic material model, as it is similar to values of 0.2% proof stress obtained from tensile testing of Type 321 stainless steels, as discussed in Section 6.2.4. The Ramberg-Osgood nonlinear elastic-plastic material model (Equation 13, described in Section 5.3.2) was used to define the stress-strain curve in these analyses. Parameters used in the model are summarised in Table 14. Two different hardening exponents were assumed for the current work ($n = 5$ and 10), which are representative of steels of interest. The hardening exponent of $n = 20$ was not analysed in this study, as it was for the bend specimen analyses of Section 6, because of the observation of significant plasticity for this hardening exponent. The sensitivity of the results to the choice of yield stress was not investigated.

### 7.3.4 Loads and Boundary Conditions

For the linear elastic analyses, a concentrated nodal force of 1000 N was applied to a reference point, kinematically constrained to all nodes in the model representing the location of interaction between the loading pin and the hole (assumed to be the upper $180^\circ$ arc on the surface of the hole, as shown in Figure 136).

For the elastic-plastic analyses, the magnitude of the applied load was uniquely defined for each geometry, depending on the calculated limit load for the geometry (R6 Section IV.1.5.1, using a plane strain von Mises formulation):
The applied loadings were defined to cover an approximate range of \( 0 < L_r < 2 \). This range of loading is adequate to allow appropriate load-displacement curves to be produced. All of the analyses were based on a small-strain assumption for simplicity and consistency.

Twenty loading steps (with equal increments) were defined for each elastic-plastic analysis. The models were physically constrained using a symmetric boundary condition on the crack plane, along the uncracked ligament (preventing in-plane rotation and displacement perpendicular to the crack plane), and also along the mid-plane of the geometry. It was decided not to incorporate a representation of the restraint effect due to anti-buckling plates used in the current test regime, since this could unduly affect the results and limit the transferability of the results to a more generic understanding of out-of-plane constraint behaviour. However, buckling is prevented in the modelled geometry through the symmetrical loading configuration. Applied loads and boundary conditions are shown in Figure 136 (out-of-plane symmetric boundary condition not shown, for clarity).

### 7.3.5 Crack Tip Modelling

The direction of the initiation of cracking in this case was assumed to be along the crack plane (symmetry plane), since the geometry and loading is symmetrical. However, it is noted that in reality, the direction of crack growth locally may not be along the symmetry plane (due to microstructural considerations). Crack tip parameters (\( J \) integral and \( T \) stress) were extracted along the Virtual Crack Extension (VCE) direction extending along the crack plane direction. The parameters were extracted at 20 contours extending radially out from the crack tip. It is noted that the first two contour integrals were considered to be inaccurate in providing appropriate fracture mechanics data and were therefore excluded. Careful consideration was given to the contour dependence of the crack tip parameters through the thickness of the specimen, since gradients near the surfaces can be significant due to the lower constraint. There was generally good contour independence across the range of contours selected. Elastic-plastic model outputs were extracted at the surface (\( z/B = 0.0 \)), at the mid-plane (\( z/B = 0.5 \)), and at two intermediate locations (approximately \( z/B = 0.25 \) and \( 0.125 \)).
7.4 RESULTS

7.4.1 Linear Elastic Modelling

Figure 137 and Figure 138 show the variation of $J$ integral and $T$ stress across the contour integrals (at the mid-plane) for the 3 mm thick specimen and the different crack depths studied (1000 N applied loading in each case). These figures illustrate the contour independence. The near crack-tip $T$ stresses exhibit slightly greater path dependence compared to that observed for the $J$ integral. This level of contour independence exists for the other specimen thicknesses.

Figure 139 shows the variation of $J$ integral across the specimen thickness (at the third contour integral), for the 3 mm thick specimen and the different crack depths studied (1000 N applied loading in each case). Figure 139 illustrates reasonable positional independence through the majority of the thickness, except at the free surface. A similar positional independence exists for the other specimen thicknesses modelled. Figure 140 shows the variation of $T$ stress across the specimen thickness (at the third contour integral), for the 3 mm thick specimen and the different crack depths studied (1000 N applied loading in each case). Both Figure 139 and Figure 140 show the effect of the free surfaces on the fracture mechanics parameters, and the importance of analysing contour integral values across the thickness as well as radially from the crack tip, when selecting appropriate contour values.

Figure 141 shows the variation of $J$ integral with crack depth for the different specimen thicknesses (for a 1000 N applied loading in each case). $J$ was calculated as a weighted average of the through-thickness values (based upon the third contour integral), excluding the surface element contour values. Figure 141 also includes the expected results based upon the relevant SIF solution from R6 Section IV.3.6.3 at different crack depths (with plane stress conditions assumed for calculating the $J$ integral values). Clearly, the applied stress increases as thickness decreases due to the applied load being fixed, and the trend in $J$ with $B/W$ is therefore expected. Figure 142 shows the variation of $J$ integral with crack depth (the FE derived values, and the values based on R6 Section IV.3.6.3), normalised by the reference stress for a C(T) specimen (given in R6 Section IV.1.5.1, a plane stress solution with the von Mises formulation).

Figure 143 shows the variation of $J$ integral (normalised by the value derived using R6 Section IV.3.6.3) with crack depth for the different specimen thicknesses. It is noted that the FE predicted values agree well (i.e. within 1%) with those provided in R6 for the small thickness specimens. The plane stress solution can be observed to be less appropriate as the thickness increases, noting that were plane strain conditions assumed for calculating the $J$ integral, then the analytical values would increase by a factor of $(1-\nu^2)^{-1}$. 

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These comparisons of the textbook and FE derived $J$ integral values give confidence in the FE mesh to calculate the $T$ stress parameter adequately. Figure 144 shows the variation of $T$ stress with crack depth (for a 1000 N applied loading in each case). The value of $T$ stress was calculated as a weighted average of the through-thickness values (based upon the third contour integral), excluding the surface element contour values. Since applied stress increases as thickness decreases (due to the applied load being fixed), the trend in $T$ with $B/W$ is expected. Figure 145 shows the variation of $T$ stress normalised by the uncracked applied stress, with crack depth, for comparison with the values as calculated by Kfouri [169]. The FE values calculated here are seen to be comparable to those calculated by Kfouri using 2D plane strain finite element analysis (with the difference thought to be due to the different notch shapes in the current and Kfouri [169] analyses).

Figure 146 shows the variation of $\beta_T$ with crack depth, for different specimen thicknesses, which was derived using the reference stress solution for a C(T) specimen (given in R6 Section IV.1.5.1, a plane stress solution with the von Mises formulation). In-plane geometric constraint values increase slightly as the specimen thickness decreases, but are positive in all cases. At $a/W = 0.5$, $\beta_T = 0.39$ for $B = 19$ mm and $\beta_T = 0.48$ for $B = 2$ mm. The fact that the in-plane geometric constraint curves do not lie on top of one another implies that there is a transition from plane stress to plane strain behaviour as the specimen thickness increases. $\beta_T$ values derived from the analyses are summarised in Table 16 along with the crack tip parameters.

One important point to acknowledge is that in reality, components fail by plastic collapse as well as fracture and it is important to consider both failure mechanisms in any fracture assessment. To illustrate the interaction between the two failure mechanisms for this geometry and setup, $K_r$ and $L_r$ parameters for each configuration were plotted on Failure Assessment Diagrams (FADs), based on an Option 1 Failure Assessment Curve (FAC). Figure 147 and Figure 148 show the FADs for a 19 mm thick and 3 mm thick specimen respectively. $L_r$ was based on the calculated limit load for the geometry (from R6 Section IV.1.5.1, a plane stress solution with the von Mises formulation) and a 0.2% proof stress of 300 MPa. The $L_r$ cut-off value was based on a tensile strength of 450 MPa. $K_r$ was based upon the elastic SIF for the geometry (from R6 Section IV.3.6.3) and an initiation fracture toughness of 100 MPa√m. The values of $L_r$ at fracture are seen to increase, as the $a/W$ ratio of the specimen increases. These FADs (which are not constraint modified) demonstrate that there is no significant change in the dominance of fracture or plastic collapse on the failure mechanism with a change in specimen thickness (at least using the material properties chosen).
7.4.2 Elastic-Plastic Modelling

7.4.2.1 Load-Displacement Behaviour

Figure 149 shows the variation of $J$ integral across the contour integrals (at the mid-plane) and normalised by the value at the tenth contour integral (0.01 mm from the crack tip), for the 3 mm thick specimen and a sample of the load steps ($n = 5$). Figure 149 illustrates the dependence on contour selection as loading increases. The contour dependence is due to the increase in plastic deformation around the crack tip, with a smaller proportion of the plastic zone contained within the initial contour integrals. A similar contour dependence exists for all the other specimen thicknesses and ligament ratios. For the analyses which used a material hardening exponent of $n = 10$, this contour dependence increased as shown in Figure 150 (due to the increased effect of plasticity). To be consistent, the tenth contour value will be used in all analyses to derive the $J$ integral.

Figure 151 shows the variation of $J$ integral across the specimen thickness normalised by the mid-plane value (using the tenth contour integral) for the 3 mm thick specimen and for a sample of the load steps ($n = 5$). Figure 152 shows a similar variation for the 3 mm thick specimen using a material hardening exponent of $n = 10$. These figures illustrate the positional dependence through the thickness of the specimen, due to the move towards a plane stress state on the free surface. This dependence exists for all specimens and crack depths, at all load steps, and is more significant than that observed in the linear elastic analyses. These figures also illustrate why it is important to consider a number of points through the thickness in order to fully understand the response of the specimen to loading.

Table 17 summarises the crack tip parameters of load-line displacement (LLD) and total $J$ integral extracted from a selection of the analyses ($a/W = 0.5$ and $n = 5$). The $J$ integral is a weighted average of the through-thickness values (based upon the tenth contour integral), excluding the surface element contour values, and the displacement was based upon the load-line displacement at the mid-plane (the difference between the mid-plane and free surface displacement was minimal in all cases).

Load-displacement curves were derived for each configuration. Sample load-displacement curves are shown in Figure 153 for the 3 mm thick specimen ($n = 5$) and in Figure 154 for the 3 mm thick specimen ($n = 5$), at the various crack depths.

Figure 155 shows the load-displacement curve for the 19 mm thick specimen ($n = 5$), with an $a/W$ ratio of 0.5, with the load-displacement curves that would be expected for plane stress and plane strain configurations, derived from the EPRI handbook for elastic-plastic loading [44]. Figure 156 shows a similar plot for the 3 mm thick specimen ($n = 5$) with an $a/W$ ratio of 0.5. Figure 157 shows
the J-integral versus load curve for the 19 mm thick specimen \((n = 5)\), with an \(a/W\) ratio of 0.5, with the J-integral versus load curves that would be expected for plane stress and plane strain configurations (derived from the EPRI handbook [44]). Figure 158 shows a similar plot for the 3 mm thick specimen \((n = 5)\) with an \(a/W\) ratio of 0.5. Figure 155 to Figure 158 show that the FE predicted values fall between the values derived using the EPRI equations [44], and it is possible to observe the transition towards plane stress behaviour as the thickness decreases. Similar transitions are observable for the \(n = 10\) analyses.

The results of the elastic-plastic modelling can be used to calculate \(\eta_p\) values as discussed in Section 2.3.4.1. Equation 19 may be rearranged to give an estimate for \(\eta_p\), as described by Equation 108. \(\eta_p\) can be found easily through linear regression of this equation. Figure 159 shows an example of the \(\eta_p\) values calculated for the 19 mm thick specimen \((n = 5)\), for the varying crack depths. Figure 160 shows an example of the \(\eta_p\) values calculated for the 3 mm thick specimen \((n = 5)\), for the varying crack depths. \(J_p\) was calculated by subtracting the elastic \(J_e\) (calculated from R6 Section IV.3.6.3, assuming plane strain conditions) from an average of the through-thickness values of Abaqus-calculated values of \(J\) (based upon the tenth contour integral), excluding the surface element contour values. \(U_p\) was based upon the displacement at the mid-plane (the difference between the mid-plane and free surface load-line displacement was negligible in all cases).

Figure 161 shows variations of \(\eta_p\) values versus \(a/W\), for the different thickness specimens \((n = 5\) analyses), and Figure 162 shows variations of \(\eta_p\) values versus \(a/W\), for the different thickness specimens \((n = 10\) analyses). ASTM E399 [31] proposes the following solution for \(\eta_p\) for C(T) specimens, derived using 2D plane-strain FE analyses, based on LLD:

\[
\eta_p^{LLD} = 2 + 0.522 \frac{W - a}{W}
\]

Davies et al. [170] used 2D plane stress and plane strain analysis and suggested that a value of \(\eta_p = 2.2\) would be appropriate as a mean line fit, independent of crack length. Since these estimates do not include any dependence on thickness or hardening exponent, they yield different \(\eta_p\) values than those predicted in the current analyses, but can be observed to be close to the values predicted for the 19 mm thick specimen. Equation 115 is plotted in Figure 161 and Figure 162 for comparison with the \(\eta_p\) values derived in the current analyses.

The \(\eta_p\) values calculated for the thinner specimens are significantly reduced compared to those suggested for use with plane strain specimens (calculated using 2D plane strain analyses). These
revised $\eta_p$ values should be used in fracture mechanics testing of thinner C(T) specimens to derive $J$ integral values at fracture and hence effective fracture toughness values.

### 7.4.2.2 In-Plane Constraint

A two-dimensional modified boundary layer (MBL) model was used in the previous study of thin width bend specimens (Section 6) to investigate the relationship between the crack depth, material hardening exponent and the elastic-plastic crack tip constraint.

The MBL model was set up as a semi-circle with a large radius ($r = 1000$ mm) to ensure small scale yielding (SSY). Only one half of the MBL model was required due to symmetrical loading in the specimen models. The MBL analysis was carried out for a range of applied loadings (different $J$ values) with zero $T$ stress, to obtain the SSY normalised opening stress curve. Figure 163 is a plot of the normalised opening stresses for a range of applied loadings against the distance ahead of the crack tip, normalised by crack driving force, $r/J\sigma_y$, for the SSY solution with a hardening exponent of $n = 5$, and Figure 164 is the SSY solution with a hardening exponent of $n = 10$. These SSY curves were used as reference curves for calculation of a $Q$ parameter. This $Q$ parameter is calculated based upon the difference between the SSY normalised opening stress and the normalised opening stress from the actual geometry (see Equation 28).

It was identified that the normalised opening stress field for the first load step in each analysis (i.e. the near-elastic loading) was approximately equivalent to the SSY solution, and for simplicity of calculation in the stress results manipulation, the stresses from the first load step were used to calculate the $Q$ parameter.

Component stresses from each of the specimens analysed were extracted ahead of the crack tip, for each of the twenty loading steps in each analysis. The opening stresses from the analyses were normalised and plotted against the normalised distance parameter. A sample of these plots for two of the loading configurations ($n = 5$) are presented in Figure 165 ($B = 19$ mm, $a/W = 0.5$) and Figure 166 ($B = 3$ mm, $a/W = 0.5$). These figures illustrate how the normalised stresses can deviate away from the SSY stresses as loading increases (with the $J$ integral converted to the non-dimensional loading parameter $J/(\alpha \sigma_y)$). There is increased deviation from the SSY curve in thinner specimens, for similar normalised $J$ loadings. Similar comparisons can be made for the analyses with a material hardening exponent $n = 10$, with Figure 167 ($B = 19$ mm, $a/W = 0.5$) and Figure 168 ($B = 3$ mm, $a/W = 0.5$).

$Q$ parameters were only derived for load steps which did not invalidate the assumptions of the equation. Load steps with high $J$ integral values, where the $r = 2J/\sigma_y$ value would be greater than
the length of the ligament, were excluded. Load steps with low $J$ values, where the $r = 2J/\sigma$ value would be smaller than the radial position of the second contour integral, and therefore invalid, were excluded.

The $Q$ parameters are plotted against the normalised $T$ stress in Figure 169 for the 3 mm thick specimen, for $n = 5$ (values calculated at the mid-plane position). Figure 169 shows that the crack depth does not have that much effect on the relationship between $Q$ and normalised $T$-stress, except at high normalised $T$-stress values. Figure 170 shows the relationship between the $Q$ and normalised $T$-stress for the range of thicknesses (for an $a/W$ value of 0.5, $n = 5$, using values calculated at the mid-plane). Figure 170 shows that the thickness has a significant effect on the relationship between $Q$ and normalised $T$-stress. It is worth noting that the calculated values of $T$ are positive, yet the corresponding values of $Q$ are negative, due to the reduction in normalised parameter $r(J/\sigma)$ with increased applied load. Similarly, Figure 171 shows the relationship between the $Q$ and normalised $T$-stress for the range of thicknesses (for an $a/W$ value of 0.5, $n = 10$, using values calculated at the mid-plane). The higher hardening exponent causes reduced $Q$ values for the same $T$-stress value.

$J$ integral values are plotted against the $Q$ parameters in Figure 172, for different specimen thicknesses (with $a/W = 0.5$, $n = 5$, at the mid-plane), to establish $J$-$Q$ loci which may be helpful in determining effective fracture toughness. Similar plots could be generated for other $a/W$ values. Similarly, Figure 173 shows the relationship between the $Q$ and $J$ integral for the range of thicknesses (for an $a/W$ value of 0.5, $n = 10$, using values calculated at the mid-plane). The higher hardening exponent causes increased $J$ integral values for the same $Q$ value.

### 7.4.2.3 Out-of-Plane Constraint

$T_Z$ parameters were derived ahead of the crack tip (according to the formulation in Equation 31), and plotted against the normalised distance parameter $r(J/\sigma)$. A sample of these plots for two of the loading configurations are presented in Figure 174 ($B = 19$ mm, $a/W = 0.5$, $n = 5$, mid-plane position) and Figure 175 ($B = 3$ mm, $a/W = 0.5$, $n = 5$, mid-plane position). Once a $T_Z$ parameter was calculated to be less than zero at a point ahead of the crack tip, it was assumed that full loss of out-of-plane constraint had occurred. Thinner specimens are seen to have an increased reduction in $T_Z$ with a commensurate increase in loading. Similar plots can be produced for the analyses with a material hardening exponent of $n = 10$, as shown in Figure 176 ($B = 19$ mm, $a/W = 0.5$, $n = 10$, mid-plane position) and Figure 177 ($B = 19$ mm, $a/W = 0.5$, $n = 10$, mid-plane position).
T	extsubscript{Z} parameters were then extracted at the r = 2J/\sigma, location, as with the derivation of Q. If the T	extsubscript{Z} value was negative at this distance it was assumed to be invalid and excluded. Load steps with high J integral values, where the r = 2J/\sigma value would be greater than the length of the ligament, were excluded. Load steps with low J integral values, where the r = 2J/\sigma value would be smaller than the radial position of the second contour integral, and therefore invalid, were excluded.

Plots of T	extsubscript{Z} values versus J integral values, extracted at the r = 2J/\sigma, location for different thicknesses are shown in Figure 178 (with a/W = 0.5, n = 5, at the mid-plane) and Figure 179 (with a/W = 0.5, n = 5, at the mid-plane), demonstrating the reduction in the triaxial stress ahead of the crack in the thinner specimens, and consequently the increased loss of out-of-plane constraint. Similar plots could be generated for other a/W values.

These figures illustrate how the T	extsubscript{Z} field ahead of the crack tip deviates away from the initial field as loading increases, due to a reduced triaxial stress at the crack tip under a given load. The figures also show the increased deviation in the field for thinner specimens, as the loading increases, implying an increased loss of out-of-plane constraint for thinner specimens. It is worth noting that the calculated values of T	extsubscript{Z} are positive, yet a parameter equivalent to Q (for characterising the loss of constraint) i.e. the T	extsubscript{Z} value ahead of the crack tip minus the plane strain T	extsubscript{Z} value of 0.5, would always be negative. T	extsubscript{Z} values decrease from 0.5 to 0.0 with increased plasticity, since the out-of-plane stress does not increase by an equivalent amount to the sum of the in-plane stresses.

Another measure of triaxiality, R, is the ratio of mean (hydrostatic) stress, \sigma_m, to equivalent (von Mises) stress, \sigma_{eq}:

\[
R = \frac{\sigma_m}{\sigma_{eq}}
\]

Using this measure, triaxiality fields can be plotted for the different loading configurations. The triaxiality fields from the analyses were plotted against the normalised distance parameter r/(J/\sigma). A sample of these plots for two of the loading configurations (for n = 5) are presented in Figure 180 (B = 19 mm, a/W = 0.5, at the mid-plane) and Figure 181 (B = 3 mm, a/W = 0.5, at the mid-plane). These figures illustrate how triaxiality reduces as the loading increases. They also show the increased reduction in triaxiality with loading in the thinner specimen, for a similar normalised J loading. Similar plots can be produced for the analyses with a material hardening exponent of n = 10, as shown in Figure 182 (B = 19 mm, a/W = 0.5, n = 10, at the mid-plane) and Figure 183 (B = 19 mm, a/W = 0.5, at the mid-plane).
The trends of the triaxiality parameter $R$ and the $T_z$ parameter with increased loading or a change in specimen thickness are seen to be comparable at least under the situations analysed.

### 7.4.3 Damage Modelling

#### 7.4.3.1 Ductility Exhaustion

It was assumed for the purposes of this analysis, that ductile fracture initiation can be described through a ductility exhaustion approach, where the accumulated plastic equivalent strain eventually leads to sufficient ductility exhaustion to initiate failure (corresponding to the critical growth and coalescence of voids in the material). The incremental damage, $\Delta D$, for a given incremental load, is calculated by the ratio of the accumulated plastic equivalent strain during the increment, $\Delta \varepsilon_{pl}$, to the strain to failure (fracture ductility, $\varepsilon_f$):

$$\Delta D = \frac{\Delta \varepsilon_{pl}}{\varepsilon_f}$$

Accumulation of equivalent plastic strain during the loading was determined ahead of the crack tip at a location of 0.05 mm. Sensitivity to this chosen position has not been investigated. The fracture ductility was based upon a Rice and Tracey [83] type formulation, similar to Equation 38, where it is a function of triaxiality (in this case $R = \sigma_m/\sigma_{eq}$) and material dependent constants $C_n$:

$$\varepsilon_f = C_1 + C_2 \exp \left( C_3 \frac{\sigma_m}{\sigma_{eq}} \right)$$

For multi-axial stress states, the fracture ductility is not equal to the uniaxial fracture ductility. It is dependent upon the relative magnitude of hydrostatic tension. The EDF Energy impact assessment procedure, R3 [171], reports values for four structural steels in multi-axial states measured by Hancock and Mackenzie [172] and Nash and Cullis [173], which show a reduction in ductility from that observed under uniaxial tension (triaxiality ratio of 0.33) to that under high hydrostatic tension. This trend is shown in Figure 184. The ductile failure model of Johnson and Cook [174] indicated that the ductility continues to rise as the triaxiality reduces below 0.33, though there was evidence from Teng and Wierzbicki [175] indicating a more complex situation – where the rupture strain falls when triaxiality reduces from a state of uniaxial tension to that of pure shear and then rises again when triaxiality goes from pure shear to uniaxial compression.

The triaxiality versus ductility curve used in this indicative analysis is shown in Figure 185, and used material constants of $C_1 = 0.0$, $C_2 = 2.0$, $C_3 = -1.5$. These constants were chosen to yield realistic values of fracture toughness for the indicative analysis and provide a curve comparable to
that of Figure 184. This model does not take into account onset of damage due to shear band localisation. It is assumed that this is of much less significance than the nucleation, growth and coalescence of voids. For very small thicknesses, and at the free surfaces, the shear criterion may become more dominant. An extension to this analysis could include this criterion.

When available, data from testing of C(T) specimens which displays an increase in apparent fracture toughness for a range of thicknesses, should be used to allow the constants of this damage model to be calibrated for a particular material. This could be achieved by tuning the failure prediction model (Equation 118) to match the test failure, such that for a calculated critical J integral, for each test specimen, the failure model would predict an accumulated damage of 1. This would allow a fracture toughness versus thickness relationship to be generated.

Figure 186 and Figure 187 show the accumulated damage with increased loading based on this damage formulation, for a 19 mm thick specimen and 3 mm thick specimen respectively (both with $a/W = 0.5$, $n = 5$). It was found that there was little dependence of damage accumulation in the predicted critical J integral on the $a/W$ ratio, as expected. These figures show that accumulation of critical damage occurs more readily at the mid-plane, which is where the out-of-plane constraint and triaxiality is highest. Also, the 3 mm thick sample exhibits a reduced amount of accumulated damage compared to the 19 mm thick specimen, for the same applied J integral. Figure 188 shows the accumulated damage with increased loading for all thicknesses studied (at the mid-plane, with $a/W = 0.5$, $n = 5$), illustrating a clear thickness dependence on damage accumulation.

Figure 189 and Figure 190 provide similar comparisons for the $n = 10$ analyses. In these analyses, there is less of a dependence of damage accumulation on the thickness of the specimen (and apparent fracture toughness even appears slightly lower for the thinner specimens, for the defined model characteristics defined). The reason for this, is that for the $n = 10$ analyses, the ratio of plastic strain developed ahead of the crack tip in the 3 mm specimens, to that in the 19 mm specimen, is higher than that developed in the $n = 5$ specimens. For the $n = 10$ analyses, the triaxiality is of less importance in the damage model of Equation 118, than the developed plastic strain.

It is noted that the analysis of triaxiality above indicated that both the measures of $\sigma_m/\sigma_{eq}$ and $T_z$ are adequate in describing the multi-axial stress state, and the damage model could likely be altered to be based on the $T_z$ parameter. This analysis could form part of further work.

### 7.4.3.2 Fracture Toughness Scaling

As shown above, the appropriateness of the damage model is dependent on the susceptibility of the particular material to work hardening and accumulation of plastic strain.
However, it was shown that the variation in accumulated damage due to thickness for a given loading, could be used to derive simple fracture toughness scaling models. Critical $J$ integral values, $J_C$, were derived from the various analyses (based upon the mid-plane value, for the $a/W = 0.5$ and $n = 5$ analyses), and a relationship between fracture toughness and thickness was derived. Fracture toughness was expressed using the standard relationship between $J_C$ and effective fracture toughness, $K_J$, given in Equation 52.

Figure 191 shows a plot of the predicted effective mid-plane fracture toughness versus thickness curve, and the effect of varying the material constants used in the damage model. These curves are relatively insensitive to $a/W$ for the range of geometries investigated in this work. Table 18 shows a summary of the effective fracture toughness values predicted for the different fracture ductility models used. In this indicative analysis the apparent fracture toughness values of the thin C(T) specimens are in the order of 10% to 20% greater than for the standard thicknesses.

This method would be of use for providing a toughness scaling equation for inclusion in R6. Based on the sample material-dependent constants analysed, it can be seen that fourth-order polynomials (as a function of thickness, $B$) are a reasonably good fit to the predicted effective fracture toughness values. A thickness-dependent fracture toughness, $K_{ZC}$, is therefore proposed, of the form:

$$K_{ZC} = \max(K_{IC}, a_1 + a_2B^1 + a_3B^2 + a_4B^3 + a_5B^4)$$

where the $a_n$ polynomial coefficients are constructed based on the thickness versus effective fracture toughness curve. A database of these coefficients could be constructed from analysis of different material dependent constants, $C_n$, using Equation 111. Table 19 shows a summary of the $a_n$ polynomial coefficients for the material-specific ductility curves assessed.

### 7.5 DISCUSSION

#### 7.5.1 Comparison with Data from the Literature

The scarcity of data regarding the effect of out-of-plane constraint loss on the apparent fracture toughness of steels that fail by a ductile fracture mechanism makes it difficult to validate the model generated in this study. As data becomes available, the model can be refined to ensure that it predicts the variation of fracture toughness with thickness and becomes a useful fracture toughness scaling model.
However, the trend of the thickness effect on apparent fracture toughness can be observed in data that is available for steels that operate in the DBT region. As highlighted in Section 6.5.1, Rathbun et al. [168] assessed in-plane constraint loss for a typical low alloy pressure vessel steel (A533B steel) in the DBT transition region, to identify increases in apparent fracture toughness. Some of this data was manipulated and is shown in Figure 131. There is clearly an effect on apparent fracture toughness from the specimen thickness. The data have therefore been re-plotted as Figure 192 to illustrate the effect of thickness more clearly.

Hudson and Newman [176] studied the effect of specimen thickness on the fatigue crack growth and fracture behaviour of 7075-T6 and 7178-T6 aluminium-alloy sheet, with specimen thicknesses ranging from 5.1 mm to 12.7 mm for 7075-T6 and 1.3 mm to 6.4 mm for 7178-T6. These aluminium grades were in common use at the time of the study for many aerospace structures. The specimens used were centre cracked tension (CCT) specimens, 292 mm wide and 889 mm long, with the longitudinal axes of the specimens parallel to the rolling direction of the material. The data that was collected by Hudson and Newman is plot in Figure 193 and Figure 194 for the Al7075-T6 and 7178-T6 specimens respectively. There is an observable thickness effect for these aluminium grades, with the thinner specimens causing higher apparent fracture toughness values, i.e. the trend predicted by the current model.

7.5.2 Technical Outcomes

The modelling carried out during this study has allowed the following improvements in technical understanding:

- An appreciation of the variance in elastic and elastic-plastic in-plane and out-of-plane geometric constraint in varying thicknesses of C(T) specimens.

- More detailed definitions of plastic eta factor, and their dependence on thickness, crack depth, and material hardening exponent than provided in the literature. These relationships should be used to assist with the analysis of thin C(T) specimens.

- $\textit{J-Q}$ loci created which will be of use in understanding correlations between $J$ and $Q$ during testing of different thickness specimens.

- Testing of thin C(T) specimens will allow characterisation of increased apparent fracture toughness, if tensile properties are sufficient to prevent plastic collapse.

- Out-of-plane constraint factor seen to be a reasonable estimator of the reduction in triaxiality in a specimen leading to increased fracture ductility and subsequent increased apparent fracture toughness.
A damage model and toughness scaling model were developed to characterise the enhanced apparent fracture toughness in a smaller thickness C(T) specimen. The models can be calibrated to provide a relationship between thickness and apparent fracture toughness, depending on the specific material of interest.

### 7.6 CONCLUSIONS

Fracture mechanics parameters ($J$ integral, elastic $T$ stress, elastic-plastic in-plane constraint parameter $Q$, and the proposed out-of-plane constraint parameter $T_Z$) were derived for C(T) specimens under various loading configurations using finite element analysis. $\eta_p$ factors were derived for different specimen thicknesses, and the dependence upon $a/W$ analysed. The $\eta_p$ factors, which are more detailed than those provided in the literature, may be used to derive critical $J$ integral values during fracture toughness testing of thin C(T) specimens. The $\beta_T$ constraint factor was derived for different thicknesses of C(T) specimens. The analysis shows that thinner specimens have comparable in-plane constraint to standard thickness specimens. The proposed $T_Z$ parameter was shown to provide a reasonable description of the out-of-plane constraint loss in the thinner specimens for the different configurations, and the subsequent increase in apparent fracture toughness. Trends can also be inferred from the relationship between elastic $T$ stress and the elastic-plastic $Q$ parameter at different thicknesses, with the relationship for thinner specimens deviating from the relationship for more standard thicknesses. $J$-$Q$ loci were created which will be of use in understanding correlations between $J$ and $Q$ during testing of different thickness specimens.

A damage model based on the ductility exhaustion approach was employed to estimate the critical $J$ integral value at the initiation of ductile fracture in the various configurations. A ‘Rice and Tracey’ type formulation was used to describe the relationship between the crack tip triaxiality and the fracture ductility. For an assumed set of damage model constants, a relationship exists between the thickness of the specimens and the predicted critical value of $J$ integral at the initiation of ductile fracture. Further work may be able to calibrate the damage model and toughness scaling models developed for these analyses, to estimate different material responses and subsequent apparent fracture toughness values.

There is an indication that thin C(T) specimens will have a higher effective fracture toughness than the thicker specimens. However, it should be noted that two-parameter approaches to fracture mechanics are known to break down under large scale yielding conditions, and three-parameter approaches may also have reduced validity in these circumstances. Prediction of increased apparent fracture toughness is only useful for specimens with sufficiently high tensile properties,
otherwise plastic collapse is more likely to be the dominant failure mode. It is important to consider each potential failure mechanism in any fracture assessment.

7.7 SUGGESTED FUTURE WORK

The modelling contained in this study may support ongoing fracture mechanics tests of thin C(T) specimens at EDF Energy. There is an indication that thin specimens will have a higher effective fracture toughness than the thicker specimens.

This study summarises a method that could be used to predict the increase in effective fracture toughness for thin specimens, if the relationship between fracture ductility and triaxiality for the material in question is understood. Further analysis using this approach may be desirable to provide estimates of increased fracture toughness based on different fracture ductility curves. These curves could be calibrated through fracture toughness tests of specimens with a range of thicknesses.

Some advice could be provided, in the form of a section for inclusion in R6, describing a simplistic process for formulating a fracture toughness scaling equation. A sample fracture toughness scaling equation may also be provided, given some sample data, in the form of a worked validation example.

It is worth noting that the proposed damage model is based upon the failure mechanism of the growth of a void reaching a critical size (leading to ductile fracture), and does not consider any other failure mechanisms (such as shear band localisation). An alternative damage model may be required under the circumstances of a different failure mechanism being dominant.

Refinements to the damage model used could also be based on the out-of-plane constraint parameter, $T_z$, if this is appropriate for data that becomes available. Analysis of this refinement to the method could form part of further work.

Future work could also investigate constraint behaviour in thin section specimens with significant welding residual stresses, and subsequently include analysis of the effects of weld mismatch and residual stresses on crack tip constraint.
## 7.8 TABLES

<table>
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<tr>
<th>Sample ID</th>
<th>Start Crack Length (mm), $a_0$</th>
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*Note* – (*) specimens cut to 3 mm thick from 19 mm thick rolled plate. Other specimens cut from 3 mm rolled plate. LT/TL = longitudinal/transverse, transverse/longitudinal direction.

Table 14: Fracture Toughness Testing of AISI Type 321 Plate [157]
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Table 15: Ramberg-Osgood Parameters
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Note – $T$ Stress and SIF values are based on the through-thickness weighted average of the third contour integrals, excluding the surface element contour integral values. $\beta_T$ values are calculated based upon a plane stress reference solution with von Mises formulation.

**Table 16 : Fracture Mechanics Parameters Extracted from Linear Elastic Analyses of C(T) Specimens (Applied Load of 1000 N)**
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<td>2.76</td>
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**Note** – LLD is the load-line displacement at the mid-plane. $J$ is the through-thickness average of the tenth contour integrals, excluding the surface element contour integral values.

**Table 17 : Parameters Extracted from a Sample of Elastic-Plastic Analyses of C(T) Specimens ($a/W = 0.5$, $n = 5$)**
### Table 18: Predicted Effective Fracture Toughness ($K_{JC}$) using Different Fracture Ductility Models, Assuming Plane Strain Behaviour for all Thicknesses (see Figure 191), $n = 5$

<table>
<thead>
<tr>
<th>$B$ (mm)</th>
<th>Predicted Effective Fracture Toughness, $K_{JC}$ (MPa√m)</th>
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<tr>
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<td>$C_1 = 0.0$, $C_2 = 2.0$, $C_3 = -1.5$</td>
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<tr>
<td>2</td>
<td>146.8</td>
</tr>
<tr>
<td>3</td>
<td>142.9</td>
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<td>4</td>
<td>139.7</td>
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<td>5</td>
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<td>10</td>
<td>129.6</td>
</tr>
<tr>
<td>19</td>
<td>126.6</td>
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</table>

**Note** – Effective fracture toughness values based on mid-plane values, with $a/W = 0.5$. Accumulated damage based upon a location 0.05 mm from the crack tip.

### Table 19: Sample Polynomial Coefficients for Toughness Scaling Equation

<table>
<thead>
<tr>
<th>$a_n$</th>
<th>Polynomial Coefficients for Toughness Scaling Equation</th>
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<tr>
<td>4</td>
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</tbody>
</table>

**Note** – Toughness scaling equation of the form $K_{JC} = (a_0 + a_1B^1 + a_2B^2 + a_3B^3 + a_4B^4)$, where $B$ is the thickness of the specimen.
**7.9 FIGURES**

Figure 132: C(T) Standard Test Geometry from BS7448-1 [32]

*B* is the thickness

*W* is the effective width

*W* = 2*B* (see 5.1)

Total width, *C* = 1.25*W* min.

Half height, *H* = 0.6*W*

Hole diameter, *d* = 0.25*W*

Half distance between holes, *h* = 0.275*W*

Crack length, *a* = 0.45*W* to 0.55*W*

Surface finish is in micrometres.
Figure 133: Fracture Toughness Test Data [157]
Figure 134: Sample of the C(T) Meshes Used in the FE Analyses (Quarter Symmetry Models), a) $B = 3$ mm, $a/W = 0.5$, b) $B = 19$ mm, $a/W = 0.5$
Figure 135: Sample of the C(T) Meshes Used in the FE Analyses – Crack Tip Close-Up

Figure 136: Boundary Conditions in the FE Analyses

Load Applied to Reference Point (Kinematically Coupled to Loaded Contact Surface Directly Above)

Free Surface

Vertical Constraint (Symmetry Plane)

Mid-Plane (Symmetry Plane)
Figure 137: Linear Elastic Analysis – $J$ Integral (At Mid-Plane) versus Contour Number
($B = 3$ mm, Applied Loading = 1000 N)

Figure 138: Linear Elastic Analysis – $T$ Stress (At Mid-Plane) versus Contour Number
($B = 3$ mm, Applied Loading = 1000 N)
Figure 139: Linear Elastic Analysis – $J$ Integral (Third Contour Integral) versus Distance Along Crack Front ($z/B = 0$ at Surface) ($B = 3$ mm, Applied Loading = 1000 N)

Figure 140: Linear Elastic Analysis – $T$ Stress (Third Contour Integral) versus Distance Along Crack Front ($z/B = 0$ at Surface) ($B = 3$ mm, Applied Loading = 1000 N)
Figure 141: $J$ Integral (Third Contour Integral Averaged Through-Thickness, Excluding Surface Element Values) versus $a/W$ (Comparison with R6 Section IV.3.6.3) – Linear Elastic Analysis (Applied Loading $= 1000$ N)

Figure 142: Normalised $J$ Integral, $J/\sigma_{ref}$ (mm) versus $a/W$ (Comparison with R6 Section IV.3.6.3) – Linear Elastic Analysis
Figure 143: \( J \) Integral (Third Contour Integral Averaged Through-Thickness, Excluding Surface Element Values) Normalised by R6 Section IV.3.6.3 Derived Value, versus \( a/W \) – Linear Elastic Analysis

Figure 144: \( T \) Stress (Third Contour Integral Averaged Through-Thickness, Excluding Surface Element Values) versus \( a/W \) – Linear Elastic Analysis (Applied Loading = 1000 N)
Figure 145: $T$ Stress (Third Contour Integral Averaged Through-Thickness, Excluding Surface Element Values) Normalised by Uncracked Applied Stress versus $a/W$ – Linear Elastic Analysis (Comparison with Kfouri [169] Values)

Figure 146: $\beta_T$ (Evaluated using $T$ Stress Values Averaged Through-Thickness, Excluding Surface Element Values) versus $a/W$
Figure 147: Failure Assessment Diagram, \( B = 19 \text{ mm} - K_{\text{MAT}} = 100 \text{ MPa} \sqrt{m}, \sigma_Y = 300 \text{ MPa} \)

Figure 148: Failure Assessment Diagram, \( B = 3 \text{ mm} - K_{\text{MAT}} = 100 \text{ MPa} \sqrt{m}, \sigma_Y = 300 \text{ MPa} \)
Figure 149: $B = 3$ mm, $a/W = 0.5$ – Elastic-Plastic Analysis – $J$ Integral (At Mid-Plane) versus Contour Number, Normalised by the Tenth Contour Value, for a Sample of Load Steps, $n = 5$

Figure 150: $B = 3$ mm, $a/W = 0.5$ – Elastic-Plastic Analysis – $J$ Integral (At Mid-Plane) versus Contour Number, Normalised by the Tenth Contour Value, for a Sample of Load Steps, $n = 10$
Figure 151: $B = 3$ mm, $a/W = 0.5$ – Elastic-Plastic Analysis – $J$ Integral Normalised by Mid-Plane Value (Based Upon Tenth Contour Integral) versus Distance Along Crack Front ($z/B = 0$ at Surface), $n = 5$

Figure 152: $B = 3$ mm, $a/W = 0.5$ – Elastic-Plastic Analysis – $J$ Integral Normalised by Mid-Plane Value (Based Upon Tenth Contour Integral) versus Distance Along Crack Front ($z/B = 0$ at Surface), $n = 10$
Figure 153: $B = 3$ mm, Load-Displacement (LLD) Curves (At Mid-Plane), $n = 5$

Figure 154: $B = 3$ mm, Load-Displacement (LLD) Curves (At Mid-Plane), $n = 10$
Figure 155: $B = 19$ mm, $a/W = 0.5$, $n = 5$, Load-Displacement Curves (At Mid-Plane). Results shown for FE and EPRI Solutions [44] for Plane Stress and Plane Strain.

Figure 156: $B = 3$ mm, $a/W = 0.5$, $n = 5$, Load-Displacement Curves (At Mid-Plane). Results shown for FE and EPRI Solutions [44] for Plane Stress and Plane Strain.
Figure 157: $B = 19$ mm, $a/W = 0.5$, $n = 5$, $J$-Integral (Averaged Across Thickness) versus Load. Results shown for FE and EPRI Solutions [44] for Plane Stress and Plane Strain.

Figure 158: $B = 3$ mm, $a/W = 0.5$, $n = 5$, $J$-Integral (Averaged Across Thickness) versus Load. Results shown for FE and EPRI Solutions [44] for Plane Stress and Plane Strain.
Figure 159: Derivation of Plastic Eta ($\eta_p$) Factor from Linear Regression of Normalised Plastic Work (Averaged Through-Thickness, Excluding Surface Element Values) and Displacement (At Mid-Plane) ($B = 19$ mm, $n = 5$)

Figure 160: Derivation of Plastic Eta ($\eta_p$) Factor from Linear Regression of Normalised Plastic Work (Averaged Through-Thickness, Excluding Surface Element Values) and Displacement (At Mid-Plane) ($B = 3$ mm, $n = 5$)
Figure 161: $\eta_p$ versus $a/W$ for the Range of Specimen Thicknesses Studied – Normalised Plastic Work Averaged Through-Thickness and Load Line Displacement at Mid-Plane, $n = 5$

Figure 162: $\eta_p$ versus $a/W$ for the Range of Specimen Thicknesses Studied – Normalised Plastic Work Averaged Through-Thickness and Load Line Displacement at Mid-Plane, $n = 10$
Figure 163: Normalised Opening Stresses ($\sigma_{22}/\sigma_0$) for SSY Solution with $T = 0$ MPa (Different Applied $J$ Integral Loadings), $n = 5$

Figure 164: Normalised Opening Stresses ($\sigma_{22}/\sigma_0$) for Different Applied $T/\sigma_0$ Values
Figure 165: Normalised Crack Opening Stresses ($\sigma_{22}$) at the Mid-Plane for Sample Geometry ($B = 19$ mm, $a/W = 0.5$, $n = 5$) for Derivation of $Q$ Parameter and Comparison with SSY Stresses

Figure 166: Normalised Crack Opening Stresses ($\sigma_{22}$) at the Mid-Plane for Sample Geometry ($B = 3$ mm, $a/W = 0.5$, $n = 5$) for Derivation of $Q$ Parameter and Comparison with SSY Stresses
Figure 167: Normalised Crack Opening Stresses ($\sigma_{22}$) at the Mid-Plane for Sample Geometry ($B = 19$ mm, $a/W = 0.5$, $n = 10$) for Derivation of $Q$ Parameter and Comparison with SSY Stresses

Figure 168: Normalised Crack Opening Stresses ($\sigma_{22}$) at the Mid-Plane for Sample Geometry ($B = 3$ mm, $a/W = 0.5$, $n = 10$) for Derivation of $Q$ Parameter and Comparison with SSY Stresses
Figure 169: Normalised $T$ Stress versus $Q$ parameter at Mid-Plane ($B = 3$ mm, $n = 5$)

Figure 170: Normalised $T$ Stress versus $Q$ for Range of Thicknesses at Mid-Plane
$(a/W = 0.5, n = 5)$
Figure 171 : Normalised $T$ Stress versus $Q$ for Range of Thicknesses at Mid-Plane
($a/W = 0.5, n = 10$)

Figure 172 : $J$ Integral versus $Q$ for the Range of Thicknesses at the Mid-Plane
($a/W = 0.5, n = 5$)
Figure 173: $J$ Integral versus $Q$ for the Range of Thicknesses at the Mid-Plane

(a/W = 0.5, n = 10)

Figure 174: $T_z$ Parameter at the Mid-Plane for Sample Geometry ($B = 19\text{mm}, a/W = 0.5$, $n = 5$) for a Range of Applied Loads
Figure 175: $T_z$ Parameter at the Mid-Plane for Sample Geometry ($B = 3$ mm, $a/W = 0.5$, $n = 5$) for a Range of Applied Loads

Figure 176: $T_z$ Parameter at the Mid-Plane for Sample Geometry ($B = 19$ mm, $a/W = 0.5$, $n = 10$) for a Range of Applied Loads
Figure 177: $T_Z$ Parameter at the Mid-Plane for Sample Geometry ($B = 3$ mm, $a/W = 0.5$, $n = 10$) for a Range of Applied Loads

Figure 178: $J$ Integral versus $T_Z$ for the Different Thicknesses of Specimen at the Mid-Plane ($a/W = 0.5$, $n = 5$)
Figure 179: $J$ Integral versus $T_2$ for the Different Thicknesses of Specimen at the Mid-Plane
($a/W = 0.5, n = 10$)

Figure 180: Triaxiality ($R$) versus Normalised Distance ahead of the Crack Tip ($B = 19$ mm,
$a/W = 0.5, n = 5$, at Mid-Plane) for a Range of Applied Loads
Figure 181: Triaxiality ($R$) versus Normalised Distance ahead of the Crack Tip ($B = 3$ mm, $a/W = 0.5$, $n = 5$, at Mid-Plane) for a Range of Applied Loads

Figure 182: Triaxiality ($R$) versus Normalised Distance ahead of the Crack Tip ($B = 19$ mm, $a/W = 0.5$, $n = 10$, at Mid-Plane) for a Range of Applied Loads
Figure 183: Triaxiality ($R$) versus Normalised Distance ahead of the Crack Tip ($B = 3$ mm, $a/W = 0.5$, $n = 10$, at Mid-Plane) for a Range of Applied Loads

Figure 184: Fracture Ductility versus Triaxiality for Sample of Structural Steels [172, 173]
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Figure 186: Accumulated Damage (B = 19 mm, a/W = 0.5, n = 5)
Figure 187: Accumulated Damage ($B = 3$ mm, $a/W = 0.5$, $n = 5$)

Figure 188: Accumulated Damage Comparison Across Range of Thicknesses Studied ($a/W = 0.5$, $n = 5$)
Figure 189: Accumulated Damage ($B = 19$ mm, $a/W = 0.5$, $n = 10$)

Figure 190: Accumulated Damage ($B = 3$ mm, $a/W = 0.5$, $n = 10$)
Figure 191: Effective Fracture Toughness ($K_{JC}$) versus Thickness based on Varying Damage Model Parameters, $n = 5$. $K_{JC}$ Calculated Assuming Plane Strain for all Thicknesses.

Figure 192: Variation in Apparent Fracture Toughness with Specimen Width for Charpy Specimens [168]
Figure 193: Variation in Apparent Fracture Toughness with Crack Length and Specimen Thickness for Al7178-T6 CCT Specimens [176]

Figure 194: Variation in Apparent Fracture Toughness with Crack Length and Specimen Thickness for Al7075-T6 CCT Specimens [176]
8. FURTHER DISCUSSION – DEVELOPMENT OF DEFECT TOLERANCE ASSESSMENT METHODS

8.1 OVERVIEW

The methods, analyses and tools developed during this EngD and presented in this thesis, could be used to provide enhancements to defect tolerance assessment procedures, by incorporating a reduction in the inherent conservatisms. As components in nuclear plant become older and degrade, challenges need to be made to the assumptions of the original safety case, to permit continued operation.

The main issue with most defect tolerance assessments is that they generally employ a strictly deterministic lower bound approach. However, this thesis has demonstrated that there may be significant benefit in using methods which provide probabilistic, localised, and configuration-specific assessments. Steel components contain significant variability in effective fracture toughness, due to either material considerations (macroscopic or microstructural), or geometrical considerations including the effect of crack tip constraint.

This work was originally carried out to develop methods for use with components in the nuclear industry, due to its unique challenges surrounding the material degradation of metallic components in harsh environments and complex loading situations. However, the methods will be equally applicable in other industries.

This section discusses the technical advances that have been made and presented in this thesis that should be considered for development of R6 and other defect tolerance assessment methods.

8.2 VALIDATION AND GENERAL EXPLOITATION

The advances made will increase the understanding of the fracture behaviour of steels under conditions of significant material and constraint variation. The results of the research have been used to produce benchmark methodologies and should be used to support future safety cases. In addition to the improved mechanistic understanding, tailored software tools have been developed to improve the modelling of material behaviour and provide simplistic advice for the reduction of
conservatisms. The models and software tools will allow improved assessment methodologies to be developed, enabling more cost-effective design and analysis of metallic components (potentially leading to plant life extension).

By developing the methods contained within this thesis, the first step has been taken to incorporate some useful advice into the R6 assessment procedure as well as other defect tolerance and structural integrity assessment procedures which share its principles. In order to continue this process, further validation of the models and the predictive tools contained in this thesis will need to take place, to identify the limits of validity for the guidance and ensure that a potential user does not incorrectly extrapolate any advice. This will require testing of specimens with a wide range of material properties and geometrical configurations, supported by additional modelling of these configurations. These additional tests can then be used to further calibrate the developed models and predictive tools, allowing simplistic, rigorous advice to be written for the relevant assessment procedures.

The work contained within this thesis, and carried out over the duration of the EngD, has provided Frazer-Nash Consultancy with an enhanced fracture mechanics capability, and has helped to promote the company as a technical developer of defect tolerance assessment methodologies. The company is better placed to assist with technical activities supporting the latest developments to these methodologies. The skills and knowledge gained over the course of the EngD will be used in the future to permit the company to identify more ‘systems-like’ approaches to the assessment of defect tolerance, aside from the conventional analyses that are carried out according to the various codes and standards. Frazer-Nash are at the cutting-edge of research and development in areas such as this, and the research contained in this thesis will provide another platform for further developing this area of the business in the future.

8.3 THE MASTER CURVE AND ADJUSTMENT OF EFFECTIVE DRIVING FORCE

The analysis of fracture toughness test data from standard specimens is often based upon the assumptions of planar crack fronts and homogenous material properties, since this allows for the simplified manipulation of data. However, these assumptions do not hold true for all test geometries or real components. Therefore, the first objective of the work contained in this thesis was to develop predictive tools, validated against data from the literature, which identify improvements that could be made to the estimation of fracture toughness.

A software tool was created to allow the user to make a simplified assessment of the interaction between localised material behaviour and localised geometrical effects (constraint). The main
feature of this tool takes advantage of the nature of the ductile-to-brittle transition regime of fracture toughness, where there is significant scatter in fracture toughness values derived at a particular temperature (due to the weakest link effect). This scatter allows a probabilistic element to be introduced to the tool, yielding the likelihood of the component failing under a particular load.

For a postulated defect and a given loading configuration, this leads to a probabilistic prediction of the location of fracture initiation, and a less conservative estimate of failure load, which can be used to derive an increased effective fracture toughness for the analysed component. This has led to providing an improved understanding of the likely locations of cleavage failure in geometries with complex defect shapes, which will be used for evaluation of in-service defectiveness. Probabilistic arguments for the expected failure loads will also be of use in safety case arguments.

Aspects of the tool (such as the enhanced effective fracture toughness) compare favourably to similar methods for assessing enhanced effective fracture toughness in the cleavage regime, as discussed in Section 5.6.1.1, such as the conventional constraint-modified fracture toughness approach of Ainsworth and O’Dowd [147], and under certain circumstances does not require full understanding of the Beremin $m$ value (which may not be known). Trends in increasing fracture toughness with reducing constraint are comparable to those predicted by the constraint-modified fracture toughness curve.

It was difficult to fully validate improved fracture toughness data for components with unusual defect geometries, since test specimens are generally based on well understood geometries with planar crack fronts and high constraint conditions, to facilitate calculation of a fracture toughness value, and data on unusual defect geometries in the literature are scarce. However, analysis of ‘POR’ specimens of 22NiMoCr37 steel, carried out by Keim [153], showed a similar loss of constraint and subsequent increase in effective fracture toughness to that observed in the development of this predictive tool, when comparing bend specimens with planar crack fronts to those with semi-elliptical surface defects.

This tool would be useful in terms of providing confidence (to an appropriately justified level) that a component would not fail under a certain loading with a postulated complex defect (see Figure 58 to Figure 63 for some examples). This provides a more favourable argument in comparison to a more traditional assessment, where using a lower bound assumption for the fracture toughness based on the Master Curve methodology as defined in the ASTM standard [109], a bounding treatment of other local material effects which affect fracture toughness, coupled with a conservative estimate of the effect on driving force (based on the most highly constrained and stressed area around the crack front) would yield poor defect tolerance.
The second main feature of the output from this tool allows the user to identify the more likely failure positions on a crack front with a complex shape (see Figure 58 to Figure 63 for some examples). This would enable the analyst to concentrate non-destructive evaluation effort on the more critical areas of the defective component, or to make modifications to the loading regime such that the burden is more equally shared among regions of a component with postulated defectiveness, which are less likely to be the initiating point for any fracture. Once again, validation of these failure location predictions is difficult, given the lack of available data for unusual defect geometries. Development of the prediction tool would therefore benefit from supporting examples which identify fracture initiation in unusual locations.

The tool has the capability for the user to input user-defined information for the localised material properties and geometrical information for complex defect shapes (that cannot be compared to finite element analysis that underpins some of the optimised hard-coded calculations). Further development and validation of the tool to account for more complex situations would be desirable, to allow the analyst to simulate as many configurations as possible.

### 8.4 HETEROGENEITY PREDICTION TOOL

A review of heterogeneity in datasets and their application to the calculation of more representative fracture toughness values identified that there are simple methods which may provide more accurate and potentially less conservative fracture toughness values, for steels operating in the brittle-to-ductile transition regime of fracture toughness, than those derived using conventional methods.

A second software tool was therefore created to allow a more thorough assessment of heterogeneity in fracture toughness test datasets, in order to provide more relevant fracture toughness values for defect tolerance assessments. This heterogeneity may exist as bimodal heterogeneity (perhaps due to sampling of materials with discrete differences in material characteristics, such as the sampling of a welded component, where the weld, parent material and heat affected zone may have different fracture toughness values). The heterogeneity may also be more randomly distributed, due to a continuous variability of microstructure, or due to conditions that could affect microstructure, such as irradiation embrittlement.

The tool provides indications of the level of heterogeneity in the provided dataset, and where fracture toughness values derived are different to those that would be derived using the standard Master Curve methods in the ASTM standard [109]. The inputs required for use of this tool are no more extensive than those which would be created as a result of standard fracture toughness testing, and therefore the effort required on the part of the analyst is minimal. Additional
functionality is also built into the tool, permitting an assessment of the influence of measurement uncertainty on the heterogeneous fracture toughness values derived, when such information for the various input parameters is known. The effects of measurement uncertainty on derived fracture toughness values can be monitored simplistically, or Monte Carlo analyses may be carried out based upon these measurement uncertainties, to improve probabilistic estimates of the heterogeneous fracture toughness values. If probabilistic methods are permitted for a given safety case, then these refined estimates of fracture toughness would yield less conservative defect tolerance assessments.

This tool would be useful in terms of providing increased confidence that a material (for which the dataset is representative) is less likely to fail than were the fracture toughness to be based on lower bound assumptions for the fracture toughness based on the Master Curve methodology as defined in the ASTM standard [109]. If probabilistic methods are permitted for a given safety case, then refined estimates of a more representative fracture toughness would yield less conservative defect tolerance assessments.

The tool was validated for the ‘EURO dataset’, as summarised by Heerens and Hellman [155], and it was found to provide similar estimates of heterogeneity as some similar methods incorporated into an assessment methodology by Lucon and Scibetta [154]. One of the major benefits of the methods developed in support of this thesis is that the methods allow the analyst to manipulate the relevant input data to include the effects of measurement uncertainty, and to observe the effects on the output values. For a given set of measurement uncertainties, an improved estimate of the fracture toughness for the dataset may be provided, which gives an extra dimension to the probabilistic assessment of the dataset. To understand the effect of the uncertainty, a probabilistic assessment would need to be performed, where the mean values obtained using a large number of Monte Carlo iterations would be expected to be close to those found using no uncertainties.

Further validation of the predictive tools and the enhanced measurement uncertainty analysis would be desirable to increase the confidence in these tools for use in industrial applications. This validation could take place for a wide range of datasets of different steels with fracture toughness in the cleavage regime.

8.5 THE THIN-WIDTH BEND SPECIMEN AS A FRACTURE TOUGHNESS TEST SPECIMEN

Another objective of this thesis was to confirm the viability or otherwise of a thin-width bend specimen, for characterising in-plane constraint and its effect on the apparent fracture toughness of components.
Finite element analyses were performed to assess the constraint behaviour in a bend specimen with small in-plane dimensions, and whether this specimen would be appropriate for characterising the improvement in effective fracture toughness in components with loss of in-plane constraint. The analyses did not identify the influence of constraint on the material resistance to fracture, instead focusing on the influence of the effects of structural constraint on the crack driving force. The results of the finite element analyses were validated where possible, against results from similar computational models and other advice in the literature, and the models were judged to be capable of providing adequate estimates of the parameters of interest.

The elastic in-plane structural constraint factor was derived for different specimen widths of bend specimens, and the analysis showed that different width specimens generally have comparable elastic in-plane constraint. However, the elastic-plastic in-plane structural constraint factor was also derived, and the analysis showed that thinner width specimens have reduced elastic-plastic in-plane constraint.

Correlations between the different constraint parameters and the $J$ integral were found, which supported previous work on similar geometries, but would be of use in understanding data from testing of thin width bend specimens. The analyses indicate that testing of thin width bend specimens will allow characterisation of increased apparent fracture toughness for specimens with sufficiently high tensile properties (weaker tensile properties may mean that plastic collapse is more likely to be the dominant failure mode).

Relationships were also developed between the applied load and crack mouth displacement at fracture, which deviate from the suggested relationships in the standard, especially for shallower defects. The relationships developed in this work have a clear explicit dependence on specimen width for shallower defects (where in-plane constraint loss is significant), which is not included in the simplified relationships defined in the standard (due to the assumption of deeply cracked specimens). The enhanced relationships should be used to assist with testing of thin-width bend specimens in future testing programmes, and will also help to inform the discussion as to how two-parameter fracture mechanics is implemented in everyday defect tolerance assessment.

The results of these analyses were compared to some testing of bend specimens of A533B steel, studied by Hadley and Karger [167] and Rathbun et al. [168], under different constraint conditions, which showed that the effective fracture toughness values increased above the plane strain fracture toughness value under conditions of low in-plane constraint. The tests were more relevant for assessing the effect of crack tip constraint on cleavage fracture, although it was found that thin width bend specimens were generally found to be acceptable for material types with high strengths (some ferritic steels). However, there is comparability between the geometric constraint.
parameters calculated in these studies and those performed as part of the thesis, with a demonstration of the subsequent effect on apparent fracture toughness.

Further validation of the conclusions of this phase of work would be desirable, with testing of austenitic steel components with low in-plane constraint (but with higher strengths than those tested in support of the work in this thesis) corroborating the increases in fracture toughness.

### 8.6 Fracture Toughness Scaling to Account for the Thickness Effect

Finally, the concept of out-of-plane constraint loss (i.e. the thickness effect) and its effect on apparent fracture toughness was studied through the analysis of thin compact tension specimens. Finite element analyses were performed to assess the constraint behaviour in thin compact tension specimens, and whether these specimens would be appropriate for characterising the improvement in effective fracture toughness in components with loss of out-of-plane constraint. The results of the finite element analyses were validated against results from similar computational models, other advice in the literature, and experimental data where possible. The models were judged to be capable of providing adequate estimates of the parameters of interest.

The elastic in-plane structural constraint factor was derived for different thicknesses of compact tension specimen, and the analysis showed that different thickness specimens generally have different elastic in-plane constraint. The elastic-plastic in-plane structural constraint factor was also derived and the analysis showed that thinner specimens have reduced elastic-plastic in-plane constraint. A proposed out-of-plane constraint parameter was shown to provide a reasonable description of the out-of-plane constraint loss in the thinner specimens for the different configurations, indicating an associated increase in apparent fracture toughness.

Correlations between the different constraint parameters and the $J$ integral were found, which supported previous work on similar geometries, but would be of use in understanding test data from testing of thin compact tension specimens. The results of these analyses were compared to some testing of thin compact tension specimens by Rathbun et al. [168] and Hudson and Newman [176], which showed that effective fracture toughness values increased above the plane strain fracture toughness value under conditions of low out-of-plane constraint.

Relationships were also developed between the applied load and crack mouth displacement at fracture, which deviate from the suggested relationships in the standard, especially for shallower defects. The relationships developed in this work have a clear explicit dependence on specimen thickness, which is not included in the simplified relationships defined in the standard (due to the
assumption of deeply cracked plane strain specimens). The enhanced relationships should be used to assist with testing of thin compact tension specimens in future testing programmes.

A damage model based on the ductility exhaustion approach was employed to estimate the critical $J$ integral value at the initiation of ductile fracture in the various configurations. In the model, an understanding of the relationship between the crack tip triaxiality and the fracture ductility (with an assumed set of model constants) was found to allow a prediction of a relationship between the thickness of the specimens and the predicted critical value of $J$ integral at the initiation of ductile fracture. It was demonstrated that a database of fracture toughness scaling curves could be constructed based on material-specific damage model constants.

The scarcity of data regarding the effect of out-of-plane constraint loss on the apparent fracture toughness of steels that fail by a ductile fracture mechanism makes it difficult to validate the damage model generated in this study. As data becomes available, the model can be refined to ensure that it predicts the variation of fracture toughness with thickness and becomes a useful fracture toughness scaling model. Further validation of the damage and toughness scaling models against fracture toughness data from test specimens with various thicknesses and material properties would be desirable to allow calibration of the damage model and development of lookup tables for the relevant material-specific model constants. This model could then be used to predict subsequent apparent fracture toughness values for any thickness of component.

The analyses indicate that thin compact tension specimens will have a higher effective fracture toughness than thicker specimens. However, it should be noted that two-parameter approaches to fracture mechanics are known to break down under large scale yielding conditions, and three-parameter approaches may also have reduced validity in these circumstances. Prediction of increased apparent fracture toughness is only useful for specimens with sufficiently high tensile properties, otherwise plastic collapse is more likely to be the dominant failure mode (a hypothesis supported by the lack of increase in effective fracture toughness for the analyses that considered a softer material).
9. CONCLUSIONS

9.1 GENERAL CONCLUSIONS

The overall objective of this EngD was to develop the methodologies used in the fracture assessment of steel components, by incorporating a reduction in the conservatisms inherent in the assessment procedures. The work contained in this thesis has investigated some of the conservatisms associated with applying a 'lower bound' treatment to steel components, which in reality contain significant variability in effective fracture toughness, due to either material considerations (macroscopic or microstructural), or geometrical considerations including the effect of crack tip constraint.

This work should assist with enabling more cost-effective design and analysis of metallic components. Primarily, the work will be of interest for components in nuclear plant, due to the special challenges that metallic components face under intense loading environments, although there is no reason why the methods may not be equally applicable in other industries.

The results of the work contained in this thesis were published in peer-reviewed papers and presented at conference, over the duration of the EngD. The development of the effective driving force adjustment prediction tool was published by Kulka [177]. The analysis of the proposed thin-width bend specimen was published by Kulka [178]. The analysis of the effect of out-of-plane constraint in thin compact tension specimens was published by Kulka and Sherry [179].

9.2 SPECIFIC CONCLUSIONS

The following conclusions can be drawn from the work reported in this thesis:

- As nuclear power stations reach the end of their lives, there is a desire to refine fracture mechanics assessments to reduce some of the inherent conservatisms in the assessment of the structural integrity of the plant. A reduction of these conservatisms may enable the safe extension of the lifetime of existing plant and also allow more efficient designs of components to be created in the future.

- A method for assessing a localised effective driving force under conditions of variable constraint and material toughness around a crack front has been proposed. This method is
shown to provide comparable results to other methods for dealing with constraint effects on cleavage fracture, such as the constraint-modified fracture toughness approach.

- The above method has been codified into a predictive software tool, which uses probabilistic methods to give a user a simplistic way of predicting likely locations of fracture initiation along a crack front, and the likely failure loads, in components with fracture toughness in the ductile-to-brittle regime of fracture toughness, which has inherent scatter in fracture toughness data. This knowledge allows the engineer to concentrate testing and analysis effort on areas in the component with high probabilities of failure.

- Methods for identifying the effects of dataset and material heterogeneity on calculated fracture toughness values have been codified into a prediction tool. These allow probabilistic assessments of the effect of measurement uncertainty to be performed simplistically.

- The above tools allow less conservative fracture toughness values to be used for a defect tolerance assessment, than would usually be determined using standard methods.

- Plastic eta factors, used to estimate fracture toughness from a load-displacement curve obtained in a fracture toughness specimen test, were found to be significantly different for non-standard specimens, such that toughness would be overestimated for thinner specimens were the standard procedures to be used. Plastic eta factors as a function of crack depth ratio, thickness-width ratio and material hardening exponent have been derived.

- Trends between elastic and elastic-plastic in-plane constraint factors are comparable to those in the literature, which are dependent on material hardening, but have some additional dependence on specimen width or thickness.

- Thin compact tension specimens lead to a loss of out-of-plane constraint, which can be quantified by a proposed $T_Z$ parameter. However, there is also a loss of in-plane constraint for a given $J$-integral loading. The inclusion of an out-of-plane constraint parameter for a simple addition to the two-parameter fracture mechanics theory would therefore not be adequate.

- The loss of constraint in thin components can be quantified by a triaxiality parameter, which can be used to predict an increase in fracture toughness through the use of a damage model based on a ductility exhaustion approach. This increase in fracture toughness is consistent with observations in the literature, but needs to be calibrated to be of use in a material-specific application.

These conclusions lead to suggestions for additional work, contained in the following section.
9.3 RECOMMENDATIONS FOR FURTHER RESEARCH

9.3.1 Effective Driving Force Adjustment for Low Constraint Configurations

Further developments to the prediction tool (for accurate adjustment to effective crack driving force under conditions of low constraint) and its supporting finite element analyses, are desirable to increase its functionality and make the tool more appropriate for different configurations.

The tool would benefit from include additional hard-coded fracture mechanics data for different specimen geometries, crack front shapes and loading configurations. This could either be derived from additional (or existing) finite element analysis, or from textbook solutions. An analysis of the effect of combined loading could be useful for developing an element of non-proportionality into the tool. Inclusion of the effects of out-of-plane constraint loss would also be of use in providing more accurate representation of the thickness effect on the effective crack driving force.

The inclusion of the effects of plasticity for user-defined defect geometries, through the inclusion of elastic-plastic $J$-integral values, inclusion of elastic-plastic in-plane constraint, and an adjustment to the failure load to account for proximity to plastic collapse for analysis of materials with lower tensile properties would also be of use. Improved functionality for the tool could also look at allowing the analyst to investigate the effect of a variation of tensile properties on the effective crack driving forces and prediction of locations of failure.

9.3.2 Heterogeneity Prediction Tool

Further developments to the prediction tool (for adjustment of derived transition temperatures under conditions of dataset heterogeneity), are desirable to increase its functionality and accuracy in the estimation of fracture toughness for heterogeneous populations.

The tool would benefit from the consideration of the effect of significant amounts of ductile crack growth prior to cleavage fracture, a consideration of pre-loading effects on test specimens (such as the warm pre-stressing phenomenon), or the inclusion of a modification to the derived transition temperatures to account for the crack arrest phenomenon. Development of the underlying mathematics to account for a larger number of distinct material populations would also be useful for very large datasets.

Development of the methods used to perform statistical Monte Carlo analyses would also allow increased functionality and usability for the analyst.
9.3.3 In-Plane Constraint Analysis

The modelling contained in this part of the study will support ongoing fracture mechanics tests of thin-width bend specimens, to allow improved estimates of effective fracture toughness to be made under conditions of low in-plane constraint. Thin width bend specimens were shown to have the capacity to have a higher effective fracture toughness than thicker width specimens.

However, the analysis did not assess the influence of constraint on the material resistance to fracture, but rather focused on the influence of the effects of structural constraint on the crack driving force, and the capability of thin width bend specimens to provide accurate fracture toughness values. In order to predict the constraint sensitivity of the material and the actual increase in fracture toughness of the material using a model-based approach, it would be necessary to perform more detailed finite element analysis with failure models in the material definitions, or undertake a test programme. Further analysis may therefore be desirable to provide estimates of increased effective fracture toughness in thin width bend specimens, using an appropriate damage model.

It was considered that improved estimates of elastic-plastic in-plane constraint would be obtained, if bending-dominant large deformation was taken into account. An adjustment to the elastic-plastic in-plane constraint values obtained under conditions of large deformation could allow more extensive relationships between constraint and applied loading in thin width bend specimens to be derived.

Future work could also investigate constraint behaviour in thin section specimens with significant welding residual stresses, including analysis of the effects of weld mismatch and residual stresses on crack tip constraint. This would allow greater transferability of the testing methods and analysis to in-service components, many of which are welded.

9.3.4 Out-of-Plane Constraint Analysis

The modelling contained in this part of the study will support ongoing fracture mechanics tests of thin compact tension specimens, to allow improved estimates of effective fracture toughness to be made under conditions of low out-of-plane constraint. There is an indication that thin compact tension specimens will have a higher effective fracture toughness than thicker specimens, which follows common understanding.

This study summarises a method that can be used to predict the increase in fracture toughness, if the relationship between fracture ductility and triaxiality for the material in question is understood. Alternatively, for a defined set of material-specific parameters, a fracture toughness scaling
equation may be used. Further analysis using these approaches may be desirable to provide estimates of increased effective fracture toughness for different materials. These relationships could be calibrated through fracture toughness tests of specimens with a range of thicknesses. A database of material-specific constants could then be created for use with the proposed fracture toughness scaling equation.

It is worth noting that the proposed damage model is based upon the failure mechanism of the growth of a void at a specific distance from the crack tip reaching a critical size (leading to ductile fracture), and does not consider any other failure mechanisms (such as shear band localisation). An alternative damage model may be required under the circumstances of a different failure mechanism being dominant. Analysis of the choice of location of initiating particle would also be of interest, with the analysis being extended to assess a sample volume ahead of the crack tip, which could be used to generate a more accurate estimate of initiation of ductile fracture.

Future work could also investigate constraint behaviour in thin specimens with significant welding residual stresses, and subsequently include analysis of the effects of weld mismatch and residual stresses on out-of-plane constraint. It is already known that welding residual stress distributions are affected by the thickness of components, and it would be of interest to know how these altered distributions affect the effective fracture toughness of in-service welded components.
10. REFERENCES


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APPENDIX A

Prediction Tool – Driving Force Adjustment

USER GUIDE
A.1 OPERATION

This user guide is included with the ‘Driving Force Adjustment’ prediction tool. See Section 5.4 for a description of the prediction tool.

Operation of the prediction tool is performed in stages. A summary is provided here:

- Input of the details of the test specimen geometry, material properties and test parameters.
  Input of the test temperatures and mean and standard deviation for $T_0$ values.

- Automatic manipulation of the relevant hard-coded, or user-defined fracture mechanics data, for use in the Monte Carlo simulations. These data are used to generate effective crack driving forces at discretised positions along the crack front.

- $T_0$ and $K_{MAT}$ values are assigned to the discretised points on the crack front, based on the data provided. The localised crack driving force along the crack front is calculated for an increasing load.

- Checks are made to see if the local driving force along the crack front is greater than the local fracture toughness, or if the plastic limit load has been reached. If so, the failure details are recorded (including the failure driving force and the failure location). The calculations repeat for the next iteration, with $T_0$ and $K_{MAT}$ values around the crack front being re-initialised. The number of iterations defined by the user governs the number of times this cycle repeats.

- The outputs provided at the end of the analysis give the user an indication as to the likely locations of failure and failure load.

More detail for each of these stages of operation is provided in the following sections. A flow-chart (see Figure 55) is provided with the tool, to allow the user to understand the processes as they are being implemented and to act as a guide.
A.2 SHEETS

The tool contains three worksheets which the user may access – ‘Guidance Notes’, ‘Inputs’, and ‘Printout’. These may be accessed by clicking on the relevant worksheet tab in the tool, or by clicking the navigation buttons at the top of the each worksheet.

A.2.1 GUIDANCE NOTES

The ‘Guidance Notes’ sheet provides assistance to the user whilst the tool is being used. It contains a summary of the information provided here, with information necessary to run the calculations being provided.

A.2.2 INPUTS

The user has control over the ‘Inputs’ sheet of the tool, by entering all of the data necessary to complete the assessment. A snapshot of the ‘Inputs’ sheet is shown in Figure 56.

The following parameters may be entered by the user:

- **Title** – A descriptive name for the assessment.

- **User Name** – The name of the user.

- **Toughness Distribution** – The user is required to select either ‘Lower Bound’, ‘Mean’, ‘Upper Bound’, ‘Random’, or ‘User-Defined’. This identifies the nature of the fracture toughness data which are to be used in the tool (the value of $P$ in Equations 73 and 74). The suggested default is ‘Random’, implying that the fracture toughness probability bound is randomly selected on each iteration of the calculation. Choosing ‘User-Defined’ requires the user to define the desired probability bounds.

- **$T_0$ (Mean)** – The user is free to enter any value. A warning message will be displayed if the mean value is outside the range of -250°C to +250°C, however the analysis will be permitted. If the user wishes the mean $T_0$ value to vary across the crack front, then the word ‘User’ should be typed into this cell. $T_0$ values will need to be entered for each of the discretised points along the crack front.

- **$T_0$ (Standard Deviation)** – The user is free to enter any positive value. An error message will be displayed if the value of standard deviation is outside the range of 0°C to 50°C.

- **Geometry** – The user is required to select either ‘Ellipse’, ‘Planar’, or ‘User-Defined’. Choosing ‘User-Defined’ requires the user to define the crack geometry by discretising the crack
front in two dimensions \( (x, y) \). It also requires the user to define the effective crack driving forces for a 1 kN loading, in terms of the \( J \)-integral (in N/m) and the \( T \)-stress (in MPa). Choosing either of the other two geometry options means that the hard-coded data will be used in calculation of the effective crack driving forces (‘Ellipse’ uses the hard-coded data for semi-elliptical surface defects, ‘Planar’ uses the hard-coded data for through-thickness defects). It should be noted that the current version of the tool allows only linear elastic analysis of user-defined defects and driving forces.

- **Iterations** – The user is free to enter an integer between 1 and 10000. A pop-up message warns the user that whilst a large number of iterations will increase accuracy of the prediction, the subsequent analysis may take a long time (approximately 1 second per iteration, depending upon computer processor speed). For an initial assessment of a given configuration, it is recommended that the user select a small number of iterations (<100) to identify if there are any problems with the inputs or the resulting analysis.

- **Material Model** – The user is required to select either ‘Elastic’, ‘5’, or ‘10’. This identifies which material model should be used in the computation. It is noted that choosing the ‘Elastic’ material model may result in the analysis consistently predicting plastic collapse for a given geometry, rather than fracture. This would generally indicate that the defined geometry has low constraint, and the effective crack driving force would never reach the effective fracture toughness of the material, before plastic collapse occurred. The likelihood of plastic collapse during the analysis is based on the magnitude of the supplied (or hard-coded) limit load.

- **Temperature** – The user is free to enter any value. A warning message will be displayed if the value is outside the range of -150°C to 150°C, however the analysis will be permitted. If the user wishes the temperature to vary across the crack front, then the word ‘User’ should be entered into this cell. Temperature values can then be entered for each of the discretised points along the crack front.

- **Constraint Factor** – The user is required to select either ‘10’ or ‘12’ (in MPa/°C). This identifies the constraint correction factor that should be used in the analysis (see Section 5.2.2). ‘12 MPa/°C’ is the suggested default value, however a pop-up message suggests that it may be worth performing a sensitivity study on this value.

- **Upper Shelf Fracture Toughness** – The user is free to enter a value between 20 MPa√m and 1000 MPa√m. This input is required, since the Master Curve does not model the upper shelf of a material fracture toughness curve. If, during the assessment, the effective crack driving force reaches this value (without any part of the crack front initiating fracture, or the limit load being reached), then this will be classed as a ductile fracture, and will be recorded as such. It should be
noted that the upper shelf fracture toughness will be treated as having a fixed magnitude (not varying with temperature) for each discretised point, and there will be no statistical variation predicted. It may therefore be sensible to designate a 'lower bound' upper shelf fracture toughness for this purpose, unless there is justification for doing otherwise.

- **Depth** – The user is free to enter any value. If the user has selected ‘Ellipse’ in the geometry cell, a warning message will be displayed if the value is outside the range of 2 mm to 5 mm. If the user has selected ‘Planar’ in the geometry cell, a warning message will be displayed if the value is outside the range of 5 mm to 30 mm. If the user has selected ‘User-Defined’ in the geometry cell, this depth value will not be used in the computations.

- **Aspect Ratio** – Only relevant for the hard-coded semi-elliptical geometries. The user should enter a value between 0.5 and 2.0 for the aspect ratio, $c/a$, which defines the half-length to depth of the surface-breaking defect. If the user has selected ‘Ellipse’ in the geometry cell, a warning message will be displayed if the value is outside this range. If the user has selected any other option in the geometry cell, the value in this cell will not be used in the computations.

- **$T$-$Q$ Correlation** – This allows the user to convert the $T$-stress values to a corresponding $Q$ parameter, based on the material model chosen. The correlation for the standard 3PB geometry is based upon the work of O’Dowd and Shih [59]:

$$Q = \left[ 0.7639 \left( \frac{T}{\sigma_y} \right) - 0.3219 \left( \frac{T}{\sigma_y} \right)^2 - 0.0906 \left( \frac{T}{\sigma_y} \right)^3 \right]$$

for $n = 5$

$$Q = \left[ 0.7594 \left( \frac{T}{\sigma_y} \right) - 0.5221 \left( \frac{T}{\sigma_y} \right)^2 \right]$$

for $n = 10$

This is only relevant for the hard-coded planar defect geometries, since a correlation between $T$-stress and $Q$ parameter has not been developed for the case of a 3PB specimen with a semi-elliptical surface defect. The assumption was made that the $T$-stress parameter in Equations 81 or 82 may be substituted for the purposes of the prediction tool, with a value of $Q, \sigma$, calculated from the work of O’Dowd and Shih [59]. It should be noted that the use of the $Q$ parameter in the calculation of the modified effective crack driving force has not been validated in the original literature and should therefore be used with caution. It is recommended that a sensitivity study without this conversion be performed to observe the difference in the results.
Limit Load for User-Defined Geometries – The user is required to enter a value for the limit load. This input is required, since the hard-coded plastic limit loads for the hard-coded geometries will not necessarily be relevant for the user-defined geometry. If, during the assessment, the effective applied load reaches this value (without any part of the crack front initiating fracture), then this will be classified as a plastic collapse, and will be recorded as such.

Override Limit Load for Hard-Coded Geometry – This allows the user to override the defined limit load for the hard-coded geometries (if there is a particular reason to do so). This option may be useful if the material of concern has a much higher (or lower) yield than was assumed in the assessment, or if there is justification for using a higher limit load. Table 1 provides the hard-coded limit loads for each geometry. This option is currently only permitted for elastic analysis, since elastic-plastic fracture mechanics data have not been calculated for limit loads higher than those that have been hard-coded.

User-Defined Inputs (Based on 1 kN Loading) – If the user has previously requested that user-defined inputs should be used for geometry, driving force, temperature, or transition temperature, then these values should be entered for each discretised point. The driving forces ($J$-integral and $T$-stress) should be based upon a 1 kN applied load. The chart alongside the table graphically presents the defect shape as defined, to allow the user to validate their input. No other validation of the input data will be undertaken. Warning messages will be displayed below the table if inputs are expected but not provided. Inputs that are provided, but not expected, will be ignored in the calculations.

Other areas of the ‘Inputs’ sheet include:

- **Printout Sheet’ Navigation Button** – Takes the user to the ‘Printout’ area of the tool (see Section A.2.6).

- **‘Help’ Navigation Button** – Takes the user to the ‘Guidance Notes’ area of the tool (see Section A.2.1).

- **‘Generate Results’ Button** – Initiates the analysis. Once the analysis is finished, the user is taken to the ‘Printout’ area of the tool.

- **Progress Bar** – Shows the user how close the analysis is to completion.

**A.2.3 ELASTIC RESULTS**

The elastic FEA results are hard-coded into the spreadsheet, and contain all the data relevant to the surface-breaking semi-elliptical and through-thickness planar defects. The spreadsheet was hard-coded to select the fifth contour integral extending radially from the crack tip for extraction of
the $J$-integral and the converged $T$-stress value. Values are interpolated to provide effective crack driving forces at equal positions along the crack front i.e. through the thickness for planar defects and angular position around the crack front for surface-breaking semi-elliptical defects.

The values from the hard-coded data are then manipulated to provide the $J$-integral and $T$-stress values for the specifically defined geometry on the user input sheet, and for the applied load at the particular point in the analysis. $J$-integral values are converted into $K_J$ values, using Equation 16.

For configurations with parameter values between those analysed, linear interpolation is used in the spreadsheet to determine intermediate driving forces (which was deemed to be sufficiently accurate). For configurations outside the range of the limits of validity of the hard-coded data, there is capacity for the user to specify user-defined data to describe the geometry and effective crack driving forces.

### A.2.4 ELASTIC-PLASTIC RESULTS

The elastic-plastic FEA results are hard-coded into the spreadsheet, and contain all the data relevant to the surface-breaking semi-elliptical and through-thickness planar defects, at different load steps. The spreadsheet was hard-coded to select the fifth contour integral extending radially from the crack tip for extraction of the $J$-integral. Values are linearly interpolated to provide $J$-integral values at equal positions along the crack front i.e. through the thickness for planar defects and angular position around the crack front for surface-breaking semi-elliptical defects.

The values from the hard-coded data are then manipulated to provide the $J$-integral values for the specifically defined geometry on the user input sheet, and for the applied load at the particular point in the analysis. For applied load values between those modelled in the FE analysis, values are interpolated. Elastic-plastic $J$-integral values are then converted into effective $K_J$ values, using Equation 16.

### A.2.5 BASE CALCULATIONS

The analysis begins when the user presses the ‘Generate Results’ button on the ‘Inputs’ worksheet. The progress bar on the ‘Inputs’ worksheet provides the user with an indication of how much time is left to complete the analysis. For each of the 21 discretised points for the specified geometry, the following sequence of events takes place:

- **Load Increment Initialised** – The applied load is initialised at a small value.

- **$T_0$ value assigned** – The value of $T_0$ allocated to each discretised point is randomly assigned based upon a normal distribution about the specified mean $T_0$ value, and the standard
deviation on \( T_0 \). The random number generated in each instance is used to calculate the ‘cumulative probability’ of the \( T_0 \) value, and hence the number of standard deviations from the defined mean (e.g. a random number of 0.0808 would correspond to 8.08% cumulative probability – and hence a \( T_0 \) value of 1.4 standard deviations below the mean.

- **\( K_{\text{MAT}} \) value assigned** – The value of \( K_{\text{MAT}} \) allocated to each discretised point is calculated from the assigned \( T_0 \) value, the temperature, and the chosen probability bound \( P \) (where the upper bound \( P = 0.95 \), mean \( P = 0.5 \), lower bound \( P = 0.05 \)). A limit is placed on the \( K_{\text{MAT}} \) value so that it does not exceed the upper shelf fracture toughness value as defined by the user:

\[
K_{\text{MAT}} = \max \left[ K_{\text{USHELF}}, 20 + \left( 1 + 77 \exp \left( 0.019 \left( T - T_0 \right) \right) \right) \right] \left( \ln \frac{1}{1 - P} \right)^{0.25}
\]

- **Driving Force Calculated** – The localised driving force is calculated using Equation 96. The \( K_J \) and \( T \)-stress are calculated at each discretised point, based on the hard-coded or user-defined data, and combined with the local temperature and local \( T_0 \) values to derive the local effective crack driving force.

- **Check for Failure** – If the local driving force is greater than the local fracture toughness, then initiation is assumed to occur. If not, then the process repeats, with an increment being added to the applied loading. If the applied load is greater than the hard-coded (or user-defined) collapse load, then a prediction of plastic collapse instead of failure is made.

- **Failure Data Output** – If failure has been predicted, then the following data are recorded for this iteration: the failure load, failure \( K_J \) (defined as effective SIF in the output), failure driving force, the classification of failure, and the failure location.

- **Process Repeats** – All calculations repeat from the beginning, with \( T_0 \) and \( K_{\text{MAT}} \) values around the crack front being re-initialised. The number of iterations defined by the user governs the number of times this cycle repeats.

**A.2.6 PRINTOUT**

A sample of the output provided in the ‘Printout’ sheet is shown in Figure 57.

All relevant input and analysis data are output onto the ‘Printout’ worksheet. This worksheet contains sheets of relevant output, set up to be printed on a standard A4 page. The first page contains an area where the user may add their own comments regarding the analysis.
Graphs are produced of the $K_J$ (or effective SIF), $T$-stress and effective crack driving force along the crack front, sampled at the end of the last iteration analysed. A graph of the mean fracture toughness variation with temperature is produced, along with a view of how the fracture toughness varied across the crack front (noting that this is for a single iteration of the analysis – the crack front variation of fracture toughness is re-initialised with each iteration of the analysis). A plot of the number of failures per discretised location is superimposed onto the crack front shape.

The mean and standard deviation of the values of failure load, failure $K_J$ (or effective SIF), and effective crack driving force are calculated. The proportion of brittle/ductile/plastic collapse failures is calculated. A cumulative distribution of failure is generated based on the applied load. The $3\sigma$ value of failure load ($\sim 0.1\%$) is also calculated.
APPENDIX B

Prediction Tool – Driving Force Adjustment

MACROS
B.1 USER-DEFINED FUNCTIONS

These user-defined functions are included in the software code which supports the ‘Driving Force Adjustment’ prediction tool. See Section 5.4 for a description of the prediction tool.

Code comments in the user-defined functions are shown as italics.

B.1.1 PI
‘Returns pi

Option Explicit

Const pi = 3.14159265359

B.1.2 LOGARITHM
‘Calculates log to the base ten

Function Log10(X)
    Log10 = Log(X) / Log(10#)
End Function

B.1.3 INTERPOLATION FUNCTION
‘Linear interpolation

Function Interp(X, Y, XI, N)
    ‘X, Y are arrays of data points for function Y(X)
    ‘N is the number of data points, must be ge 2
    ‘XI is the X value for which interpolation is required
    If (XI >= X(1)) And (XI <= X(N)) Then
        i = 2
        Do Until XI < X(i)
            i = i + 1
        Loop
        X1 = X(i - 1)
        X2 = X(i)
Y1 = Y(i - 1)
Y2 = Y(i)
Slope = (Y2 - Y1) / (X2 - X1)
Interp = Y1 + Slope * (XI - X1)
Else
Interp = "Outside data range"
End If
End Function

B.2 MACROS
This VBA macro is included in the software code which supports the ‘Driving Force Adjustment’ prediction tool. See Section 5.4 for a description of the prediction tool. Code comments in the VBA macro are shown as *italics*.

B.2.1 CALCULATIONS
Sub CALCS()
'* initialise sheets and cells'
ActiveWorkbook.Unprotect
Set checkCell = Worksheets("Front page").Cells(127, 2)
If checkCell.Value = 0 Then
Application.ScreenUpdating = False
Application.ScreenUpdating = True
ActiveWorkbook.Unprotect
Application.Calculate
Worksheets("Histogram"), Range("B2:h50001").ClearContents
Set incCell = Worksheets("Base Calculations").Cells(10, 3)
incs = incCell.Value
Set progCell = Worksheets("Front Page").Cells(95, 2)
progCell.Value = 0
'* Iterative Calculations
For Counter = 2 To incs + 1
    Set progCell = Worksheets("Front Page").Cells(95, 2)
    Set resCell = Worksheets("Base Calculations").Cells(5, 1)
    resCell.Value = "0"
  .resCell.Value = "1"
    Set scaleCell = Worksheets("Base Calculations").Cells(10, 17)
    scaleCell.Value = "0.0"
    Increment = 100
    Set histaCell = Worksheets("Histogram").Cells(Counter, 2)
    Set histbCell = Worksheets("Histogram").Cells(Counter, 3)
    Set histcCell = Worksheets("Histogram").Cells(Counter, 4)
    Set histdCell = Worksheets("Histogram").Cells(Counter, 5)
    Set histeCell = Worksheets("Histogram").Cells(Counter, 6)
    Set histfCell = Worksheets("Histogram").Cells(Counter, 7)
    Set failCell = Worksheets("Base Calculations").Cells(10, 22)
    Set nofailCell = Worksheets("Base Calculations").Cells(10, 24)
    Set locCell = Worksheets("Base Calculations").Cells(10, 23)
    Set loadCell = Worksheets("Base Calculations").Cells(10, 18)
    Set ducCell = Worksheets("Base Calculations").Cells(10, 19)
    Set sifCell = Worksheets("Base Calculations").Cells(10, 20)
    Set dfCell = Worksheets("Base Calculations").Cells(10, 21)
    Set maxCell = Worksheets("Base Calculations").Cells(10, 14)
    Application.Calculate
' Iterative Calculations
    Do
        Do
            scaleCell.Value = scaleCell.Value + Increment
        ' Stop Infinite Loop
Application.Calculate

Loop Until failCell.Value = "1" Or nofailCell.Value = "1"

scaleCell.Value = scaleCell.Value - Increment

Increment = Increment / 5

Loop Until Increment < "0.1"

' Report Iteration

scaleCell.Value = scaleCell.Value + 5 * Increment
histaCell.Value = locCell.Value
histbCell.Value = loadCell.Value
histcCell.Value = ducCell.Value
histdCell.Value = nofailCell.Value
histeCell.Value = sifCell.Value
histfCell.Value = dfCell.Value
progCell.Value = Counter - 1

Next Counter

' Activate Sheets

Application.Calculate

Sheets("Front Page").Activate
ActiveSheet.Protect DrawingObjects:=True, Contents:=True, Scenarios:=True
Sheets("Printout").Activate
ActiveSheet.Protect DrawingObjects:=True, Contents:=True, Scenarios:=True
Else
Sheets("Printout").Activate
ActiveSheet.Protect DrawingObjects:=True, Contents:=True, Scenarios:=True
Sheets("Front Page").Activate
ActiveSheet.Protect DrawingObjects:=True, Contents:=True, Scenarios:=True
End If

Application.Calculation = xlCalculationAutomatic
Application.ScreenUpdating = False
Application.ScreenUpdating = True

End Sub
APPENDIX C

Prediction Tool – Heterogeneity

USER GUIDE
C.1 INPUTS

This user guide is included with the ‘Heterogeneity’ prediction tool. See Section 5.5 for a description of the prediction tool.

The ‘Inputs’ tab of the tool is where all user-defined information is entered into the relevant cells. A snapshot of this inputs area is shown in Figure 65.

A constant value for a specific parameter may be entered for all tests in a dataset by ensuring that the appropriate cell is marked ‘YES’. If different values for each parameter are appropriate for each test in a dataset, the appropriate cell is marked ‘NO’.

Measurement uncertainties may also be entered for the parameters if appropriate, as a standard deviation. If required, uncertainty values will be applied during the dataset construction as a random value for each of the individual test specimens, assuming a normal distribution of uncertainty.

Once all inputs are defined by the user, the ‘Generate Population’ button may be used, to fill out all parts of the population which have constant values across all tests. This button calls a VBA macro. Values in the population which were defined as not being constant, in addition to the fracture toughness values, will still require further definition.

C.1.1 GEOMETRY

The following details must be input:

- Specimen Thickness, \( B \) (in mm);
- Specimen Width, \( W \) (in mm);
- Initial Crack Size, \( a_0 \) (in mm).

C.1.2 MATERIAL PROPERTIES

The following details must be input:

- Young’s modulus, \( E \) (in GPa);
- Poisson’s Ratio, \( \nu \);
- Yield Stress, \( \sigma_{YS} \) (in MPa).
These material properties only affect the censoring limit for the data and do not affect the analysis in any other way, so estimated values may be appropriate.

C.1.3 TEST PARAMETERS
The following details must be input:

- Number of tests for analysis, $N$;
- Measurement uncertainty for the user-input fracture toughness values (one standard deviation, in MPa $\sqrt{\text{m}}$);
- Test temperature (in °C);
- $T_0$ shift to account for strain rate effects, (in °C);
- $T_0$ shift to account for other effects, including ageing (in °C).

C.1.4 VALIDATION DATASET
A random validation dataset may be automatically generated if desired. There is the option for a bimodal or a single mode dataset to be produced, based on Gaussian distributions (with an enforced minimum fracture toughness of 20 MPa $\sqrt{\text{m}}$). The user enters the mean and standard deviation of fracture toughness and temperature for each of the two modes. An estimate of the proportion of each mode in the dataset is also required.

Pressing either the ‘Random’ or ‘Bimodal’ buttons then initiates a VBA macro which creates a validation dataset based upon the chosen parameters.

C.1.5 ANALYSIS SETUP
Once all data have been entered by the user (or the validation dataset has been created), then the tool automatically calculates other parameters required for the analysis:

- The ligament size for each test;
- The censoring limit (according to Equation 55), and whether the fracture toughness value for the test is to be censored;
- The fracture toughness is corrected for the thickness of the specimen;
- The $T_0$ shifts for strain rate and ageing effects are turned into test-specific fracture toughness shifts;
Uncertainties are applied to each of the relevant test parameters.

Graphs are produced of the test population data (disregarding $T_0$ shifts due to ageing or strain rate effects, or adjustment due to parameter uncertainty):

- A temperature versus fracture toughness scatter plot of the data, with the minimum censoring limit;
- A cumulative probability of derived fracture toughness (only useful for a defined validation dataset);
- A cumulative probability of test temperature (only useful for a defined validation dataset).

### C.2 SINTAP LOWER TAIL ANALYSIS

The ‘SINTAP’ tab of the tool is where the ‘SINTAP Lower Tail’ Analysis is carried out, as described in Section 2.6.3. Data are automatically copied from the ‘Inputs’ tab. Pressing the ‘Solve’ button automatically performs the analysis.

The $T_0$ values in the different stages of the analysis are calculated using an iterative process. In this tool (when the ‘Solve’ button is pressed), the values of $T_0$ are found using the ‘goal seek’ function in Excel.

The calculated values of $T_0$ for the dataset are presented, with the associated uncertainty. A plot of the test population and the calculated survival probability bounds is presented. A histogram is plotted, for a sample of the population, for a visualisation of the difference between the $T_0$ value calculated for the whole dataset using Stage 1 of this method, and the $T_0$ values that would be calculated for individual tests by fitting a Master Curve through them. Examples of output are provided, using a validation dataset, in Section 5.5.4.

### C.3 BIMODAL HETEROGENEITY ANALYSIS

The ‘Bimodal’ tab of the tool is where the ‘Bimodal Heterogeneity Analysis’ is carried out, as described in Section 2.6.4. Data are automatically copied from the ‘Inputs’ tab. Pressing the ‘Solve’ button automatically performs the analysis.

The $T_0$ values for the two distributions, $T_{0A}$ and $T_{0B}$, and the probability of a specimen belonging to distribution A, $p_A$, are calculated using an iterative process. Three independent parameters make calculation of the maximum likelihood somewhat more difficult than for the single parameter in the
SINTAP lower tail analysis. In this tool (when the ‘Solve’ button is pressed), the value of $T_0$ is found iteratively, using the ‘Solver’ Add-In function in Excel to facilitate the calculations.

The calculated values of $T_{0A}$, $T_{0B}$ and $p_A$ for the dataset are presented, with the associated uncertainties. A $T_0$ estimate is also calculated for the combined dataset. A plot of the test population and the calculated survival probability bounds is presented.

A histogram is plotted, for a sample of the population, for a visualisation of $T_0$ values calculated for the whole dataset using the bimodal analysis, and the $T_0$ values that would be calculated for individual tests by fitting a Master Curve through them. Examples of output are provided, using a validation dataset, in Section 5.5.4.

C.4 RANDOM HETEROGENEITY ANALYSIS

The ‘Random’ tab of the tool is where the ‘Random Heterogeneity Analysis’ is carried out, as described in Section 2.6.5. Data are automatically copied from the ‘Inputs’ tab. Pressing the ‘Solve’ button automatically performs the analysis.

Firstly, a simple estimate is made of the Gaussian distribution of fracture toughness in the dataset, using the Single Point Estimation method. This is used as a benchmark for the more accurate maximum likelihood estimate.

The mean $T_0$ and $\sigma T_0$ values for the distribution are calculated using an iterative process. Because of the necessity to numerically integrate the survival probability and distribution functions (which are functions of $T_0$) across a large range of $T_0$ values, it was decided to solve the parameters to an accuracy of integer values (to save on computational effort), but future development of this tool could allow increased refinement.

In this tool (when the ‘Solve’ button is pressed), the values of mean $T_0$ and $\sigma T_0$ are found by iterating across a range initialised using an average of the Single Point Estimate and SINTAP Stage 1 and Stage 2 estimates as a benchmark. The calculated values of mean $T_0$ and $\sigma T_0$ are presented based upon the Single Point Estimation and Maximum Likelihood models. Plots of the test population and the calculated survival probability bounds are presented based upon both the Single Point Estimation and Maximum Likelihood models.

A histogram is plotted, for a sample of the population, for a visualisation of the difference between the $T_0$ value calculated for the whole dataset using the maximum likelihood method, and the $T_0$ values that would be calculated for individual tests by fitting a Master Curve through them. Examples of output are provided, using a validation dataset, in Section 5.5.4.
APPENDIX D

Prediction Tool – Heterogeneity

MACROS
D.1 MACROS

These VBA macros are included in the software code which supports the 'Heterogeneity' prediction tool. See Section 5.5 for a description of the prediction tool.

Code comments in the VBA macros are shown as *italics*.

D.1.1 POPULATE DATASET

Sub GenPop()

' Macro purpose - Generation of dataset, excluding toughness values and any variables chosen to be user-defined.

' Macro generates temp, thickness, width, crack size,
' modulus, poisson ratio, yield, shifts for the tab 'Inputs'.

Set Z = Worksheets("Inputs").Cells(33, 38)

If Z.Value = 1 Then

MsgBox "Some parameters incorrectly specified. Check red cells for errors."

Else

Application.ScreenUpdating = False


' How many data points?

Set incCell = Worksheets("Inputs").Cells(9, 11)

incs = incCell.Value

' Check values of constants

Set CheckA = Worksheets("Inputs").Cells(9, 36)

Set CheckB = Worksheets("Inputs").Cells(11, 36)

Set CheckC = Worksheets("Inputs").Cells(13, 36)

Set CheckD = Worksheets("Inputs").Cells(15, 36)

Set CheckE = Worksheets("Inputs").Cells(17, 36)

Set CheckF = Worksheets("Inputs").Cells(19, 36)

Set CheckG = Worksheets("Inputs").Cells(21, 36)
Set CheckH = Worksheets("Inputs").Cells(23, 36)
Set CheckI = Worksheets("Inputs").Cells(25, 36)

Set ValueA = Worksheets("Inputs").Cells(12, 13)
Set ValueB = Worksheets("Inputs").Cells(23, 13)
Set ValueC = Worksheets("Inputs").Cells(26, 13)
Set ValueD = Worksheets("Inputs").Cells(29, 13)
Set ValueE = Worksheets("Inputs").Cells(9, 21)
Set ValueF = Worksheets("Inputs").Cells(12, 21)
Set ValueG = Worksheets("Inputs").Cells(15, 21)
Set ValueH = Worksheets("Inputs").Cells(15, 13)
Set ValueI = Worksheets("Inputs").Cells(18, 13)

' Clear old data.
Worksheets("Inputs").Range("e38:e9999").ClearContents
Worksheets("Inputs").Range("f38:f9999").ClearContents
Worksheets("Inputs").Range("g38:g9999").ClearContents
Worksheets("Inputs").Range("h38:h9999").ClearContents
Worksheets("Inputs").Range("j38:j9999").ClearContents
Worksheets("Inputs").Range("k38:k9999").ClearContents
Worksheets("Inputs").Range("l38:l9999").ClearContents
Worksheets("Inputs").Range("n38:n9999").ClearContents
Worksheets("Inputs").Range("r38:r9999").ClearContents
Worksheets("Inputs").Range("s38:s9999").ClearContents

' Clear random numbers
Worksheets("Inputs").Range("w38:w5000").ClearContents
Worksheets("Inputs").Range("y38:y5000").ClearContents
Worksheets("Inputs").Range("aa38:aa5000").ClearContents
Worksheets("Inputs").Range("ac38:ac5000").ClearContents
Worksheets("Inputs").Range("ae38:ae5000").ClearContents
Worksheets("Inputs").Range("ag38:ag5000").ClearContents
For Counter = 38 To incs + 37
' Set values
  Set ACell = Worksheets("Inputs").Cells(Counter, 5)
  Set BCell = Worksheets("Inputs").Cells(Counter, 6)
  Set CCell = Worksheets("Inputs").Cells(Counter, 7)
  Set dCell = Worksheets("Inputs").Cells(Counter, 8)
  Set ECell = Worksheets("Inputs").Cells(Counter, 10)
  Set FCell = Worksheets("Inputs").Cells(Counter, 12)
  Set GCell = Worksheets("Inputs").Cells(Counter, 11)
  Set HCell = Worksheets("Inputs").Cells(Counter, 18)
  Set ICell = Worksheets("Inputs").Cells(Counter, 19)
If CheckA.Value = 1 Then
  ACell.Value = ValueA.Value
End If
If CheckB.Value = 1 Then
  BCell.Value = ValueB.Value
End If
If CheckC.Value = 1 Then
  CCell.Value = ValueC.Value
End If
If CheckD.Value = 1 Then
  dCell.Value = ValueD.Value
End If
If CheckE.Value = 1 Then
  ECell.Value = ValueE.Value * 1000
End If
If CheckF.Value = 1 Then
    FCell.Value = ValueF.Value
End If

If CheckG.Value = 1 Then
    GCell.Value = ValueG.Value
End If

If CheckH.Value = 1 Then
    HCell.Value = ValueH.Value
End If

If Check1.Value = 1 Then
    ICell.Value = Value1.Value
End If

Next Counter

For Counter = 38 To incs + 37
    ' Generate random numbers for both T and K combos, and the mode of each data point
    Set UCellR = Worksheets("Inputs").Cells(Counter, 23)
    UCellR.Value = Rnd

Next Counter

    Application.Calculate

    Application.Calculation = xlCalculationAutomatic

    Application.ScreenUpdating = False

    Application.ScreenUpdating = True
End If
End Sub

D.1.2 BIMODAL DATASET GENERATION

Sub GenBi()
    ' Macro purpose - Generation of population with bimodal heterogeneity.
Application.ScreenUpdating = False

' How many data points?
Set incCell = Worksheets("Inputs").Cells(9, 11)
incs = incCell.Value

' Clear old data.
Worksheets("Inputs").Range("w38:w5000").ClearContents
Worksheets("Inputs").Range("y38:y5000").ClearContents
Worksheets("Inputs").Range("aa38:aa5000").ClearContents
Worksheets("Inputs").Range("ac38:ac5000").ClearContents
Worksheets("Inputs").Range("ae38:ae5000").ClearContents
Worksheets("Inputs").Range("ag38:ag5000").ClearContents

' Initialise cells for each increment.
For Counter = 38 To incs + 37

' Generate random numbers for both T and K combos, and the mode of each data point
Set TCellR = Worksheets("Inputs").Cells(Counter, 27)
Set KCellR = Worksheets("Inputs").Cells(Counter, 25)
Set UCellR = Worksheets("Inputs").Cells(Counter, 23)
Set TCellR2 = Worksheets("Inputs").Cells(Counter, 31)
Set KCellR2 = Worksheets("Inputs").Cells(Counter, 29)
Set MCellR2 = Worksheets("Inputs").Cells(Counter, 33)

TCellR.Value = Rnd
KCellR.Value = Rnd
UCellR.Value = Rnd
TCellR2.Value = Rnd
KCellR2.Value = Rnd
MCellR2.Value = Rnd

Next Counter
Application.Calculate

For Count = 38 To incs + 37

' Write in toughness and temperature data into sheet. Temps only if check = 0

Set TCellX = Worksheets("Inputs").Cells(Count, 26)
Set KCellX = Worksheets("Inputs").Cells(Count, 24)
Set TCellX2 = Worksheets("Inputs").Cells(Count, 30)
Set KCellX2 = Worksheets("Inputs").Cells(Count, 28)
Set MCellR2 = Worksheets("Inputs").Cells(Count, 33)
Set TCell = Worksheets("Inputs").Cells(Count, 5)
Set KCell = Worksheets("Inputs").Cells(Count, 14)
Set Mode = Worksheets("Inputs").Cells(26, 16)

If MCellR2.Value < Mode.Value Then
    KCell.Value = KCellX.Value
Else
    KCell.Value = KCellX2.Value
End If

If CheckA.Value = 0 Then
    If MCellR2.Value < Mode.Value Then
        TCell.Value = TCellX.Value
    Else
        TCell.Value = TCellX2.Value
    End If
Else
    End If
End If

Next Count

Application.Calculation = xlCalculationAutomatic
Application.ScreenUpdating = False
D.1.3 RANDOM DATASET GENERATION

Sub GenRan()

' Macro purpose - Generation of population with random heterogeneity.
Application.ScreenUpdating = False
' How many data points?
Set incCell = Worksheets("Inputs").Cells(9, 11)
incs = incCell.Value
' Clear old data.
Worksheets("Inputs").Range("w38:w5000").ClearContents
Worksheets("Inputs").Range("y38:y5000").ClearContents
Worksheets("Inputs").Range("aa38:aa5000").ClearContents
Worksheets("Inputs").Range("ac38:ac5000").ClearContents
Worksheets("Inputs").Range("ae38:ae5000").ClearContents
Worksheets("Inputs").Range("ag38:ag5000").ClearContents
' Initialise cells for each increment.
For Counter = 38 To incs + 37
' Generate random numbers for the T and K combo
Set TCellR = Worksheets("Inputs").Cells(Counter, 27)
Set KCellR = Worksheets("Inputs").Cells(Counter, 25)
Set UCellR = Worksheets("Inputs").Cells(Counter, 23)
TCellR.Value = Rnd
KCellR.Value = Rnd
UCellR.Value = Rnd
Next Counter
Sub SINTAP()
    ' Macro purpose - Generates master curve and probability bounds based upon standard SINTAP analysis.
    ' SINTAP Lower-Tail Multi-Temperature Analysis
    Application.MaxChange = 0.00001
    ActiveWorkbook.PrecisionAsDisplayed = False
    Application.ScreenUpdating = False
    Application.ScreenUpdating = True
Next Counter
End Sub

D.1.4 SINTAP LOWER TAIL ANALYSIS

Sub SINTAP()
    ' Macro purpose - Generates master curve and probability bounds based upon standard SINTAP analysis.
    ' SINTAP Lower-Tail Multi-Temperature Analysis
    Application.MaxChange = 0.00001
    ActiveWorkbook.PrecisionAsDisplayed = False
    Application.ScreenUpdating = False
    ' Initialise search cells and clear old data
    Sheets("SINTAP").Activate

Application.Calculate
For Counter = 38 To incs + 37
    ' Write in toughness and temperature data into sheet
    Set TCellX = Worksheets("Inputs").Cells(Counter, 26)
    Set KCellX = Worksheets("Inputs").Cells(Counter, 24)
    Set TCell = Worksheets("Inputs").Cells(Counter, 5)
    Set KCell = Worksheets("Inputs").Cells(Counter, 14)
    KCell.Value = KCellX.Value
    If CheckA.Value = 0 Then
        TCell.Value = TCellX.Value
    Else
    End If
Next Counter
Application.Calculation = xlCalculationAutomatic
Application.ScreenUpdating = False
Application.ScreenUpdating = True
End If
End Sub
Set a = Worksheets("SINTAP").Cells(16, 20)
a.Value = -99
Set b = Worksheets("SINTAP").Cells(16, 25)
b.Value = -99
Worksheets("SINTAP").Range("aa38:ac9999").ClearContents
Worksheets("SINTAP").Range("y28:y28").ClearContents
' Set number of data points
Set inc = Worksheets("SINTAP").Cells(8, 3)
incs = inc.Value
' Goal seek on Stage 1 and Stage 2a MML Estimator
    Range("t17").GoalSeek Goal:=0, ChangingCell:=Range("t16")
Set T01 = Worksheets("SINTAP").Cells(27, 20)
Set T03 = Worksheets("SINTAP").Cells(28, 25)
    T03.Value = T01.Value
Set T03 = Worksheets("SINTAP").Cells(28, 25)
    T03.Value = T01.Value
    Range("y17").GoalSeek Goal:=0, ChangingCell:=Range("y16")
Set TK2 = Worksheets("SINTAP").Cells(19, 25)
Set TR2 = Worksheets("SINTAP").Cells(20, 25)
' Check Cells
Set T02 = Worksheets("SINTAP").Cells(27, 25)
    T02.Value = T01.Value
' Write out initial T0 guesses
Set WriteA = Worksheets("SINTAP").Cells(38, 27)
    WriteA.Value = 1
Set WriteB = Worksheets("SINTAP").Cells(38, 28)
    WriteB.Value = T01.Value
Set WriteA = Worksheets("SINTAP").Cells(39, 27)
    WriteA.Value = 2
Set WriteB = Worksheets("SINTAP").Cells(39, 28)
    WriteB.Value = T02.Value
Set WriteC = Worksheets("SINTAP").Cells(39, 29)
WriteC.Value = TR2.Value
Counter = 40
' Stage 2 iterations until analysis stops
Do
    Set ACell = Worksheets("SINTAP").Cells(18, 24)
    If ACell.Value = 1 Then
        T03.Value = T02.Value
        Range("y17").GoalSeek Goal:=0, ChangingCell:=Range("y16")
        Set WriteA = Worksheets("SINTAP").Cells(Counter, 27)
        WriteA.Value = Counter - 37
        Set WriteB = Worksheets("SINTAP").Cells(Counter, 28)
        WriteB.Value = T02.Value
        Set WriteC = Worksheets("SINTAP").Cells(Counter, 29)
        WriteC.Value = TR2.Value
    End If
    Counter = Counter + 1
Loop While ACell.Value = 1
Application.Calculation = xlCalculationAutomatic
Application.ScreenUpdating = False
Application.ScreenUpdating = True
Application.MaxChange = 0.001
ActiveWorkbook.PrecisionAsDisplayed = False
End Sub

D.1.5 BIMODAL ANALYSIS
Sub BimodalSolver()
' Macro purpose - Generates master curve and probability bounds based upon assumption of bimodal heterogeneity.

Application.MaxChange = 0.00001

ActiveWorkbook.PrecisionAsDisplayed = False

'Solver - SINTAP Lower Tail Analysis First - To get an estimate of the mean, sigT0
'S Then
'S Start Bimodal Analysis

Sheets("Bimodal").Activate

' Initialise search cells

Set ReadA = Worksheets("SINTAP").Cells(27, 6)
Set WriteA = Worksheets("Bimodal").Cells(24, 6)
WriteA.Value = ReadA.Value

Set ReadB = Worksheets("SINTAP").Cells(26, 6)
Set WriteB = Worksheets("Bimodal").Cells(25, 6)
WriteB.Value = ReadB.Value

Set WriteC = Worksheets("Bimodal").Cells(26, 6)
WriteC.Value = 0.5

SolverReset

SolverAdd CellRef:="$f$26", Relation:=1, FormulaText:="0.99"
SolverAdd CellRef:="$f$26", Relation:=3, FormulaText:="0.01"
SolverOptions MaxTime:=100, Iterations:=10000, Precision:=0.0005,
AssumeLinear:= _
   False, StepThru:=False, Estimates:=1, Derivatives:=1, SearchOption:=1, __
   IntTolerance:=0.005, Scaling:=True, Convergence:=0.0005,
AssumeNonNeg:=False

SolverOk SetCell:="$w$36", MaxMinVal:=1, ValueOf:="0",
ByChange:="$f$24:$f$26"

SolverSolve True

If WriteA.Value - WriteB.Value < 0.1 Then
If WriteA.Value - WriteB.Value > -0.1 Then
    WriteC.Value = 1#
    End If
End If

Application.ScreenUpdating = True

' Goal seek for toughness on survival function, with a defined probability, across temp
range.

' Iteration across temperature curve
For Counter = 38 To 68
    ' Select the first T val
    Set TCellG = Worksheets("Bimodal").Cells(33, 32)
    Set KCellG = Worksheets("Bimodal").Cells(33, 31)
    Set TCell = Worksheets("Bimodal").Cells(Counter, 32)
    TCellG.Value = TCell.Value
    Set SCellA = Worksheets("Bimodal").Cells(33, 35)
    Set SCellB = Worksheets("Bimodal").Cells(33, 36)
    Set SCellC = Worksheets("Bimodal").Cells(33, 37)
    Set SCellD = Worksheets("Bimodal").Cells(33, 38)
    Set KCellA = Worksheets("Bimodal").Cells(Counter, 33)
    Set KCellB = Worksheets("Bimodal").Cells(Counter, 34)
    Set KCellC = Worksheets("Bimodal").Cells(Counter, 35)
    Set KCellD = Worksheets("Bimodal").Cells(Counter, 36)
    Application.Calculate
    KCellG.Value = 32
    Range("ai33").GoalSeek Goal:=0.99, ChangingCell:=Range("ae33")
    KCellA.Value = KCellG.Value
    KCellG.Value = 32
    Range("ai33").GoalSeek Goal:=0.95, ChangingCell:=Range("ae33")
KCellB.Value = KCellG.Value
KCellG.Value = 32
Range("ai33").GoalSeek Goal:=0.5, ChangingCell:=Range("ae33")
KCellC.Value = KCellG.Value
KCellG.Value = 32
Range("ai33").GoalSeek Goal:=0.05, ChangingCell:=Range("ae33")
KCellD.Value = KCellG.Value
’ Goto the next T val
Next Counter
KCellG.Value = 100
Range("ai33").GoalSeek Goal:=0.5, ChangingCell:=Range("af33")
End Sub

D.1.6 RANDOM HETEROGENEITY ANALYSIS
Sub RandCalcs()
’ Macro purpose - Generates master curve and probability bounds based upon assumption of random heterogeneity.
Application.MaxChange = 0.00001
ActiveWorkbook.PrecisionAsDisplayed = False
’ Solver - SINTAP Lower Tail Analysis First - To get an estimate of the mean, sigT0
’ Then
’ Start Random Analysis - MML Estimation
Worksheets("Random").Range("am37:ba50000").ClearContents
Worksheets("Random").Range("ai38:ai50000").ClearContents
’ Total number of data points
Set incCellA = Worksheets("Random").Cells(8, 3)
incsA = incCellA.Value

' Start the standard deviation incrementation this amount below the guess
Set incCellB = Worksheets("Random").Cells(29, 40)
incsB = incCellB.Value

' Increment the standard deviation by this much
Set incCellC = Worksheets("Random").Cells(30, 40)
incsC = incCellC.Value

' How may standard deviation increments?
Set incCellD = Worksheets("Random").Cells(28, 40)
incsD = incCellD.Value

' Initialise cells for each increment.
' A = Mean, B = standard deviation
Set ACellGuess = Worksheets("Random").Cells(25, 24)
Set BCellGuess = Worksheets("Random").Cells(26, 24)
Set ACell = Worksheets("Random").Cells(32, 24)
Set BCell = Worksheets("Random").Cells(33, 24)
ACell.Value = ACellGuess.Value - 8#
' 8 is because we want to look 7 each side of the mean guess, minus 1 for initialisation

' Iteration of A - mean (15 increments)
For CountA = 39 To 53
Application.Calculate
ACell.Value = ACell + 1
If BCellGuess.Value - incsB < 0.1 Then
' There is a shift of 0.3 here, stops standard deviation of zero being analysed, which
' causes problems.
BCell.Value = 0.3 - 1#
Else: BCell.Value = BCellGuess.Value - incsB - 1#
End If

' Iteration of B - standard deviation.
For CountB = 38 To incsD + 37
BCell.Value = BCell.Value + 1

'Iteration of X - data points
For Counter = 38 To incsA + 37
'Select the first T, d and K combo
Set TCellX = Worksheets("Random").Cells(Counter, 5)
Set KCellX = Worksheets("Random").Cells(Counter, 15)
Set dCellX = Worksheets("Random").Cells(Counter, 13)
Set TCell = Worksheets("Random").Cells(30, 23)
Set KCell = Worksheets("Random").Cells(30, 24)
Set dCell = Worksheets("Random").Cells(30, 22)
Application.Calculate

TCell.Value = TCellX.Value
KCell.Value = KCellX.Value
dCell.Value = dCellX.Value

'the Likelihood Function Is calculated. Write this in.
Set LCellX = Worksheets("Random").Cells(33, 33)
Set LCell = Worksheets("Random").Cells(Counter, 35)
LCell.Value = LCellX.Value

'Goto the next T+K combo
Next Counter

'For the first increment on SD. The total likelihood has been calc'd.
Set FCellX = Worksheets("Random").Cells(CountB, CountA)
Set FCell = Worksheets("Random").Cells(33, 35)

'Screen update to show progress - can switch off if affecting performance
Application.Calculate
Application.ScreenUpdating = True
Application.ScreenUpdating = False
FCellX.Value = FCell.Value

Next CountB

Set Header = Worksheets("Random").Cells(37, CountA)
Header.Value = ACell.Value
Application.ScreenUpdating = True
Application.Calculate
Application.ScreenUpdating = False
Next CountA

Set FinalCheckA = Worksheets("Random").Cells(31, 44)
Set FinalCheckB = Worksheets("Random").Cells(32, 38)
Set FinalCheckC = Worksheets("Random").Cells(31, 39)
Application.Calculation = xlCalculationAutomatic

' Goal seek for toughness on survival function, with a defined probability, across temp range.

' Iteration across temperature curve
For Counter = 38 To 68
    Set dCell = Worksheets("Random").Cells(30, 22)
    dCell.Value = 1#

    ' Select the first T, K combo
    Set TCell = Worksheets("Random").Cells(30, 23)
    Set TCellX = Worksheets("Random").Cells(Counter, 63)
    TCell.Value = TCellX.Value
    Set KCell = Worksheets("Random").Cells(30, 24)
    KCell.Value = 32
    Set KCellA = Worksheets("Random").Cells(Counter, 64)
    Set KCellB = Worksheets("Random").Cells(Counter, 65)
    Set KCellC = Worksheets("Random").Cells(Counter, 66)
    Set KCellD = Worksheets("Random").Cells(Counter, 67)
    Application.Calculate
Range("ae33").GoalSeek Goal:=0.99, ChangingCell:=Range("x30")
KCellA.Value = KCell.Value
KCell.Value = 32
Range("ae33").GoalSeek Goal:=0.95, ChangingCell:=Range("x30")
KCellB.Value = KCell.Value
KCell.Value = 32
Range("ae33").GoalSeek Goal:=0.5, ChangingCell:=Range("x30")
KCellC.Value = KCell.Value
KCell.Value = 32
Range("ae33").GoalSeek Goal:=0.05, ChangingCell:=Range("x30")
KCellD.Value = KCell.Value
'
Goto the next T+K combo
'
Next Counter

Application.ScreenUpdating = True

End Sub