COMPUTER SIMULATION OF DIFFUSIONAL CREEP FAILURE OF ENGINEERING ALLOYS

by

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1. Summary.

A simplified model with only 2 degrees of freedom is developed for cavity growth along a grain-boundary by surface and grain-boundary diffusion following a similar model for a row of grains used by Sun et al., (1996). A variational principle for the coupled diffusion problem is used to follow the cavity growth. The approximate solution can be reduced to the well-established equilibrium cavity growth model at the fast surface diffusion extreme. By comparing the 2 degree of freedom model with the full finite element solution by Pan et al., (1997), a ‘Validity Map’ is constructed in terms of the relative diffusivity and applied stress relative to the capillarity stress. It is found that the simplified model accurately describes the evolution process, in terms of overall cavity profile and propagation rate for engineering alloys subject to normal levels of applied stresses.

The 2 degree of freedom model for a single cavity was then extended to allow the modelling of multiple cavities. These cavities can be either pre-existing or nucleated during the lifetime of the system. The relative rotation between the grains is also considered. The initial 2 degrees of freedom were increased to six, and a cavity element has been derived. The cavity elements are assembled together using the classical finite element approach. This allows the evolution of multiple cavities and their interactions to be modelled under different applied loads and material parameters.

This simplified multiple cavity finite element model was compared with a model for cavity evolution based on a ‘smeared-out’ approach. It was shown that the ‘smeared-out’ model does not accurately predict the creep damage for realistic engineering materials and conditions and results in an under prediction of creep lifetime.

Using the simplified finite element model the effect of surface diffusion on the evolution of the creep damage was investigated. The evolution of a large pre-existing ‘crack-like’ cavity was modelled and the effects of nucleation, surface diffusion and loading were also investigated. It was shown that in the majority of cases as the surface diffusion was increased the rupture time was also increased. The results from the large ‘crack-like’ cavity simulations showed that there was very little crack propagation through the material and the smaller cavities tended to grow independently of the large ‘crack-like’ cavity.
Acknowledgements.

I would like to thank my supervisors Dr J. Pan and Dr A. D. Crocombe for their patience and encouragement throughout the course of this research. Without their continuous enthusiasm during the project and the writing of this thesis I would have found it very difficult to finish it. I would also like to thank Professor A.C.F Cocks for his invaluable guidance at the beginning of this work.

Grateful acknowledgements must also go to the EPSRC for principal funding of this project as well as providing me a means to survive. Without their assistance I would not have been able to undertake a PhD.

I am also grateful to my colleagues in the solid mechanics and design research group for their general support. In particular thanks must go to Dr S. Kucherenko who provided me with invaluable assistance during the writing of the computer model and whose numerical solver saved many hours of computational time. I would also like to thank Mr S. Hill who was always there when I needed computing support.

Finally I would like to thank my parents who have continued to support and house me during my years as a student.
Declaration.

I declare that the work contained in this thesis is original and applicable to the subject area. Dr S. Kucherenko provided the numerical solver that was used in the computer program as it was far more efficient than standard solvers and significantly reduced the computation time of the model.
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<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>$A$</td>
<td>Area of cavity</td>
</tr>
<tr>
<td>$B$</td>
<td>Total height of representative unit</td>
</tr>
<tr>
<td>$B$</td>
<td>Nucleation rate constant</td>
</tr>
<tr>
<td>$b$</td>
<td>Cavity spacing</td>
</tr>
<tr>
<td>$b$</td>
<td>Burgers vector</td>
</tr>
<tr>
<td>$C$</td>
<td>Centre co-ordinate of arc</td>
</tr>
<tr>
<td>$C$</td>
<td>Constant of integration in local stress calculation</td>
</tr>
<tr>
<td>$D_s$</td>
<td>Surface diffusivity</td>
</tr>
<tr>
<td>$D_{gb}$</td>
<td>Grain boundary diffusivity</td>
</tr>
<tr>
<td>$D_v$</td>
<td>Lattice diffusion coefficient</td>
</tr>
<tr>
<td>$\delta_s$</td>
<td>Effective thickness of surface atoms involved in diffusion.</td>
</tr>
<tr>
<td>$\delta_{gb}$</td>
<td>Effective thickness of grain boundary atoms involved in diffusion.</td>
</tr>
<tr>
<td>$\delta_e$</td>
<td>Thickness of ‘smeared-out’ cavity</td>
</tr>
<tr>
<td>$\dot{\epsilon}$</td>
<td>Time dependent creep strain</td>
</tr>
<tr>
<td>$F_s$</td>
<td>Driving force of surface diffusion</td>
</tr>
<tr>
<td>$F_{gb}$</td>
<td>Driving force of grain boundary diffusion</td>
</tr>
<tr>
<td>$G$</td>
<td>Total free energy of the system</td>
</tr>
<tr>
<td>$G$</td>
<td>Shear modulus</td>
</tr>
<tr>
<td>$J$</td>
<td>Rate of nucleation of cavities per unit area and time</td>
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<tr>
<td>$J_s$</td>
<td>Surface diffusive flux</td>
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<tr>
<td>$J_{gb}$</td>
<td>Grain boundary diffusive flux</td>
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<td>$k$</td>
<td>Boltzmann’s constant</td>
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<td>$\kappa$</td>
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<tr>
<td>$l$</td>
<td>Length of uncavitated grain boundary</td>
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<td>$l_{crit}$</td>
<td>Critical length for coalescence</td>
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<tr>
<td>$M_{gb}$</td>
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<td>Free surface mobility</td>
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<tr>
<td>Symbol</td>
<td>Definition</td>
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<tr>
<td>--------</td>
<td>------------</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of cavities</td>
</tr>
<tr>
<td>$\dot{N}$</td>
<td>Rate of nucleation of cavities</td>
</tr>
<tr>
<td>$n$</td>
<td>Creep exponent</td>
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<td>$P$</td>
<td>Applied load</td>
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<td>$Q_r$</td>
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<td>$R$</td>
<td>Radius of arc forming cavity profile</td>
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<td>$R_g$</td>
<td>Molar gas constant</td>
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<td>$s$</td>
<td>Local co-ordinate along free surface</td>
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<tr>
<td>$T$</td>
<td>Absolute temperature</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$\tilde{t}$</td>
<td>Non-dimensional time</td>
</tr>
<tr>
<td>$\tau_g$</td>
<td>Reference time</td>
</tr>
<tr>
<td>$V_g$</td>
<td>Surface migration velocity</td>
</tr>
<tr>
<td>$V_{gb}$</td>
<td>Grain boundary migration velocity</td>
</tr>
<tr>
<td>$\dot{W}$</td>
<td>Rate of work done by external force</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Rotation of grain</td>
</tr>
<tr>
<td>$X$</td>
<td>Local co-ordinate along grain boundary</td>
</tr>
<tr>
<td>$x$</td>
<td>Global co-ordinate in x-direction</td>
</tr>
<tr>
<td>$x_c$</td>
<td>Global co-ordinate of cavity centre</td>
</tr>
<tr>
<td>$x_g$</td>
<td>Global co-ordinate of applied load</td>
</tr>
<tr>
<td>$Z$</td>
<td>Global x co-ordinate</td>
</tr>
<tr>
<td>$\Gamma_s$</td>
<td>Total length of free surface</td>
</tr>
<tr>
<td>$\Gamma_{gb}$</td>
<td>Total length of grain boundary</td>
</tr>
<tr>
<td>$\gamma_s$</td>
<td>Specific free energy of free surface</td>
</tr>
<tr>
<td>$\gamma_{gb}$</td>
<td>Specific free energy of grain boundary</td>
</tr>
<tr>
<td>$\sigma_n$</td>
<td>Applied stress normal to grain boundary</td>
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<tr>
<td>$\overline{\sigma}_n$</td>
<td>Normalised applied stress</td>
</tr>
<tr>
<td>$\Pi$</td>
<td>Variational functional</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>Dihedral angle</td>
</tr>
<tr>
<td>$\Psi_e$</td>
<td>Equilibrium dihedral angle</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Chemical potential</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Atomic volume</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Local x co-ordinate</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Local angle of surface</td>
</tr>
</tbody>
</table>
2. Introduction.

2.1 Historical background.

Creep resistant alloys are often required to operate at high temperatures and in the most hostile and frequently variable conditions of stress and temperature for many years. For these alloys there is a need to increase the understanding of the creep fracture process. This would allow the development of better design codes and inspection procedures that would be of particular use in high temperature applications such as electricity generating plants and petrochemical plants. With an increase in understanding of creep failure, there would come the ability to improve the material properties of high temperature alloys, which would be used in the construction of the next generation of high temperature plant.

The need for investigation into creep fracture came about after a series of catastrophic failures of power generating and petrochemical plants that have occurred in the past and have been attributed to creep fracture. The worst industrial accident in world history occurred in December 1984, when deadly methyl isocyanate gas was leaked from a chemical plant in Bhopal, India, causing the deaths of at least 3300 people. This was attributed to creep failure of the pipe work carrying the chemicals, and the subsequent release proved deadly. This shows that creep fracture is a very important part of modern day industry, which requires increased understanding.

2.2 Framework of the research program.

The purpose of this research is to develop a numerical technique to simulate the nucleation, growth and coalescence of grain boundary cavities into micro-cracks using a computer model. This process occupies most of the creep life of an engineering component, and as such is a critical factor in determining the lifetime of the component.

The first stage of the work was to develop a simplified model for cavity growth with only two degrees of freedom. Following the model for the sintering of a row of particles by
Sun et al. (1996), the cavity surface was approximated using two degrees of freedom in order to consider the full interaction between surface and grain-boundary diffusion. The second degree of freedom enabled the cavity to evolve in a non-self-similar way and highlight the effects of surface and grain boundary diffusion on cavity growth, shown in Figure 1. This model was tested and compared to a full finite element solution and found to give good results within a range of operating conditions highlighted in the 'Validity Map'. Examples of cavity evolution produced by the simplified model and compared with cavity profiles produced by the full FE model are shown in chapter 4.

![Figure 1](image-url)  
(a) Quasi-equilibrium grain boundary cavity, (b) Non-equilibrium (crack-like) cavity. $\Psi$ denotes the angle between the tangent to the cavity at the cavity tip and the x-axis (half dihedral angle), Chuang et al. (1973).

The 2 degree of freedom model was extended so that it could simulate multi-cavity growth. Six independent degrees of freedom were used to model a “cavity element” which consists of a single cavity and length of grain boundary on each side. There could be a large number of cavities present on a single grain-boundary, which would evolve and interact over time. The degrees of freedom include those describing the shape of the cavity and those describing relative motion between the cavities and grains. The cavity elements were then assembled into a global viscosity matrix for all the cavities along the grain-boundary, using the classical finite element technique. Continuous random nucleation of cavities was included in the model, as well as the ability to coalesce to form larger cavities. The user can define the material parameters and loading position, giving maximum flexibility in the types of system that can be modelled.

On completion the simplified finite element model was compared with a cavity model based on a ‘smeared-out’ approach. In this model the cavities are not modelled discretely, instead they are ‘smeared-out’ along the grain boundary. This has the advantage of being
relatively simple and requires very little processing time. The results from this model were compared to those from the simplified finite element model for a variety of operating conditions and material parameters.

In terms of justification for developing this simplified finite element model there is a clear need to develop a new model that is able to simulate all of the various types of cavity growth. The types of growth are: 'quasi-equilibrium', 'crack-like' and all the intermediate stages, without the complexity of a full finite element solution. The new model must be much faster in obtaining the remaining life assessment of the system in comparison to the full numerical solution, which can be left to run for days or even weeks at a time before the solution is reached. Previous models that have been developed were for a single cavity on a single grain boundary between two crystals. This is obviously not a realistic situation, as there can be hundreds of cavities nucleated on a single grain boundary alone. Therefore the new cavity growth model must be simple enough so that it can be integrated into the numerical technique, allowing hundreds of cavities to be nucleated and grow on a single grain boundary. At present it would be very demanding for a computer to use a full finite element model to simulate multiple cavities on a grain boundary, as the number of degrees of freedom would be enormous and the processing time would be very large.

An abridged version of the first part of this work has been published in the journal European Journal of Mechanics (Westwood et al., 2000).

2.3 Contents overview.

The principal objective of this research is to develop a simplified model that follows the evolution of multiple cavities on a grain boundary. In order to justify the need for such a model the published material in the subject area has been researched. A review of the existing literature is given in chapter 3 as well as a discussion on the importance of creep damage to industry.

Chapter 4 introduces the variational principal and the governing equations on which the 2 degree of freedom model is based. The model is then derived and the methods used for the solution of the system included. The extra modifications for fast surface diffusion are
discussed as well as the non-dimensionalisation of the expressions. Finally the model is validated with the comparisons between the 1 degree of freedom model and a full finite element model forming the basis for the 'Validity Map'. Selected cases are then presented detailing the conditions under which the model is valid and invalid.

Chapter 5 extends the model presented in the previous chapter to form the new simplified multi-cavity finite element model. The selection of the new degrees of freedom is discussed as well as the formation of the cavity ‘element’. The assembly of the elements using the classical finite element approach is performed, with the solution method outlined. Before the cavity ‘element’ is incorporated into the new model, it is validated using specially defined test cases. The cavity coalescence and nucleation mechanisms are discussed in detail, as well as the calculation of the local grain boundary stress. All of the above mechanisms are brought together at the end of the chapter in the form of a flow chart, which outlines the operational order of the computer model.

Chapter 6 introduces the ‘smeared-out’ model approach by Nguyen et al., (1998), and the general theory behind it. The damage due to nucleation has been calculated as well as the attempts made to improve the model by incorporating the 2 degree of freedom model derived during this research. A flowchart detailing the operational order of the computer program is given, followed by a discussion on the comparisons between the ‘smeared-out’ model and the simplified finite element model.

Chapter 7 investigates the effect of surface diffusion on the creep damage using the simplified finite element multi-cavity model. The results from the two different dihedral angles used are presented, as well as comparisons and conclusions.

Chapter 8 describes the ‘large-crack’ simulation. In this chapter the simplified finite element model was used to simulate a large pre-existing crack on the grain boundary. The subsequent effects of loading position, local grain boundary stress and cavity nucleation are all discussed.

Finally, chapter 9 discusses the achievements of the work as well as possible areas of further research and improvement.
3. Literature review.

3.1 Introduction.

The modelling of creep damage accumulation in engineering materials has been ongoing for more than 35 years and it has been shown that most of the creep damage occurs by the nucleation, growth and coalescence of intergranular cavities. These cavities form macrocracks, which propagate through the material to cause failure. The amount of published material relating to this topic is very large, and despite a great improvement in the understanding of these processes there is still considerable debate about the relative importance of the underlying mechanisms involved. It is inappropriate to produce a general review on the subject of creep damage accumulation here. There are a large number of books that have been written on the subject of creep damage. These include, “Cavities and Cracks in Creep and Fatigue” by Gittus (1981), “Mechanisms of Creep Fracture” by Evans (1984), “Fracture at High Temperatures” by Riedel (1987) and “High Temperature Component Life Assessment” by Webster and Ainsworth (1994). The reader is directed to these texts for a more indepth overview of the subject area.

The focus of this thesis is on the diffusional creep damage accumulation. Hence the sections in this review are limited to the areas of creep damage most relevant to the work in this thesis. There are many more publications that are related to this general subject area but they fell outside the direct scope of this work. The relevance of creep damage in an industrial environment is discussed with a brief introduction to the use of design codes for the avoidance of creep damage. The section on industrial application is completed with the inclusion of two examples of industrial projects concerning the prediction of remaining life, and an effective inspection policy to prevent catastrophic failure.

The published literature in the subject area has been broken down into four main categories: cavity nucleation models, cavity growth models, diffusional crack growth models and computer simulation of cavity and crack propagation.
3.2 Industrial relevance of creep failure.

The phenomenon of creep is not a new one as it has been observed in materials such as wood and lead pipes for centuries. Creep has only been a significant problem since the industrial revolution when the primary source of power for machinery was steam. This brought relatively high temperatures into contact with the materials of the day and creep occurred. Creep is a time dependent deformation that is most likely to occur in materials that are exposed to high temperatures and loads for an extended period of time. It is sensitive to stress and temperature and can eventually cause the failure of the material.

The relevance of creep damage to industry has been briefly outlined in the introduction, however it is a major factor in the design and maintenance of industrial plant. The industrial codes used, as well as a more detailed description of the effects of creep damage in industry is given below.

3.2.1 Industrial design procedures.

The use of design procedures limits the amount of creep damage in electric power generation equipment, chemical plants, gas turbine engines and other high temperature applications. In these applications the need for a cost effective and accurate method of avoiding failure is of great importance, as the consequences of failure could be catastrophic, such as in the nuclear industry.

There are two main considerations when designing high temperature equipment: i) avoidance of excessive creep, and, ii) prevention of fracture. These two considerations are met by the use of design codes (BSI (1989), BSI (1991), RWTÜV (1978), ASME (1990) and AFCEN (1985)). These codes give the values for maximum acceptable operating stresses and temperatures. These are dependent on the type of component and consequences of failure. An example of this would be maintaining clearance at the tip of a rotating turbine blade; therefore the design must seek to restrict the creep elongation of the blade. The design codes typically incorporate safety factors into the assessment procedures to allow for unknown conditions that may occur in the lifetime of the component, as well as variability in material properties. The magnitudes of the safety factors are determined by experience and are dependent on whether average or minimum
properties data are used. In addition different safety factors may be applied to infrequent or emergency excursions.

Most of the high temperature design codes have been developed from those that have been developed for room temperature applications. They are therefore aimed at avoiding failure by plastic collapse, fatigue and fast fracture as well as creep. It is possible to define temperatures (that vary somewhat between codes), below which creep need not be considered for particular classes of materials. An approximate guide to some of these temperatures is given in Table 3-1. More precise values should be obtained from the relevant codes.

Table 3-1. Temperatures below which creep is not usually of serious concern in boiler and pressure vessel components.

<table>
<thead>
<tr>
<th>Material</th>
<th>Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon manganese steels</td>
<td>310</td>
</tr>
<tr>
<td>Low alloy ferritic steels</td>
<td>420</td>
</tr>
<tr>
<td>Stainless steels</td>
<td>485</td>
</tr>
<tr>
<td>Alloy 800 H</td>
<td>550</td>
</tr>
<tr>
<td>Alloy 718 bolting material</td>
<td>460</td>
</tr>
</tbody>
</table>

The high temperature design codes that are currently used have been developed mainly for the use on defect-free materials. However, critical components are often now examined using non-destructive examination (NDE) methods to detect any flaws that are present. There are a variety of methods used to detect flaws such as visual, radiographic and ultrasonic inspection, depending on whether the flaws are on the surface or buried. As a result there is a need to establish a tolerance for these defects, below which no action is taken and above which repair or replacement should occur. Webster and Ainsworth, (1994), state that guidance is available for the prevention of fast fracture for elevated temperatures where creep is of concern.

Design codes are not only used at the initial design stages; they can be used to determine the condition of equipment that has been in service for a period. It is quite possible that the codes may require periodic mandatory inspections. The frequency of inspection may be different from one component to another. This can be based on past experience and...
also the consequences of failure; i.e. a more frequent inspection routine would be used on a component whose failure may be catastrophic and dangerous. Inspections of equipment can take several forms. They can be destructive or non-destructive. The actual technique used depends on the component geometry, accessibility and the nature of the damage anticipated. The method of taking plastic replicas of the component outlined by Webster and Ainsworth, (1994), to inspect the local surface texture and to determine the extent of voiding and or microcracking can be used (Figure 2).

Figure 2. Classification of creep damage in steam boilers.

Figure 2 shows how creep damage in steam boilers can be classified into four levels of severity A, B, C and D. These represent isolated creep cavities, oriented cavities, microcracks and macrocracks respectively. Depending on the level observed, the following courses of action are recommended:

- Level A: continue to operate plant but monitor damage at 3 year intervals.
- Level B: continue operation but fix inspection intervals at 1½ years.
- Level C: limited service is possible until repair.
- Level D: repair immediately.

This type of approach can be used for other materials and components provided that an accurate history of the microstructure as well as details of any cracking or damage has been maintained. Comparisons are then made between the replicas taken from the exposed material and the library of pictures to determine the remaining lifetimes. An extensive range of pictures would be needed for the different engineering alloys and to cope with the wide range of phenomena that can occur under different operating conditions.
Variation in properties between batches of material is another complication in making residual life assessments. In order to make the assessments as accurate as possible it may be necessary to make back-up measurements of properties on samples of service exposed material taken from the plant.

Many components are fabricated by welding. The welding process can pose problems because of the regions of different microstructure and because of the possible presence of residual stresses. The parent material, heat affect zone (HAZ) and weld metal can all have different creep properties. Welds are also likely sites for defects. The importance of welds in industrial plant is discussed in further detail in the next section.

3.2.2 Industrial relevance of creep damage accumulation.

The importance of creep crack propagation in industries such as power generation and petrochemical manufacture is introduced in this section. The majority of the information comes from ERA Technology who are a research, development and testing company based in Leatherhead, Surrey. ERA is an independent company that has several different divisions within it. The Plant Services Division is the one most applicable to this research as it deals with life assessment of different types of industrial plant, offering a wide range of technical services which are intended to extend the working life of these plants. ERA possesses the world’s largest independent testing laboratory that provides a long-term database and technique validation facility.

The choice of this company was made due to the fact that the author spent over a year working for them as part of his industrial training. The section contains extracts from ERA reports and proposals, which show where the industry need is, in terms of prediction of remaining life, and an effective inspection policy to prevent catastrophic failure.

3.2.3 Project A: Quantification of Creep Damage Development in Weldments.

3.2.3.1 Background.

Cracking occurs in many different locations in ferritic steel weldments including the weld metal, fusion line and heat affected zone (HAZ) of the parent metal. The actual
mechanism of cracking and the rate of damage accumulation, from one location to another, can however be vastly different. Some cracking modes, e.g. solidification cracking in the weld metal or reheat cracking in the coarse grained region of the HAZ are short term phenomena and occur during fabrication or early service. In terms of plant operation, these forms of cracking can be minimized by a proper schedule of inspection and repair and by the implementation of research findings that have achieved a broad understanding of the factors contributing to the cracking. Through this work significant improvements have been made to the metallurgical, welding and engineering aspects of weld design. The overall benefit of these improvements is however, more pertinent to welds in new plant or for repair welds. There remains a major problem of cracking in high temperature ferritic steel welds on old plant which have not benefited by the implementation of improvements in weld design. These are susceptible to the long-term degradation phenomena known as Type IV cracking.

![Figure 3a. 'Fish Mouth' failure of large bore steam pipe. Picture courtesy of ERA Technology.](image)

The root cause of Type IV cracking is predominantly microstructural. During the welding cycle, the region of the HAZ, immediately adjacent to the parent metal only attains temperatures low in the austenitic range or even in the intercritical (\(\alpha + \gamma\)) range. The result is a fine grained ferritic structure with coarsened carbides leading to a localized zone
substantially weaker than the adjacent coarse-grained HAZ, parent metal and weld metal. Type IV cracking has occurred frequently in service, examples include un-renormalised seam-welded pipe work systems in the United States, Japan and Europe e.g. (Ellis (1994), Welds (1986), Bissell et al. (1988)), and in circumferential butt welds on ferritic pipe work systems in the USA and Europe e.g. (Kimmins et al. (1993), Answald et al. (1986) and Townsend (1990)). There have been several catastrophic failures of industrial plant. Figure 3a shows a large bore steam pipe having failed in a spectacular manner.

A typical example of thermal fatigue cracking in a critical component is ‘ligament cracking’ in steam headers (Figure 3b). This form of cracking has arisen at a large number of utilities throughout Europe and the USA, and many studies have shown that ligament cracking is a result of combined effects of thermo-mechanical fatigue arising from temperature cycles and stress relaxation by creep strain during steady operation.

![Figure 3b. Classical ligament cracking between the tube penetrations in an element row. Picture courtesy of ERA Technology.](image)

One of the most intractable aspects of Type IV cracking is that because it is associated with temperatures attained during the welding cycle, all ferritic steels will show similar structures in the HAZ adjacent to the unaffected parent material. Potentially, therefore, all ferritic steels are susceptible to this form of damage albeit to a variable extent. Service experience supports this contention in that Type IV cracking has occurred in the low alloy ferritic steels 1/2CrMoV, 1-1/4Cr1/2Mo and 2-1/4CrMo, (Answald et al. (1986) and
Townsend (1990)). Cross weld laboratory rupture test data has also been obtained on all these steels, on X20 (12CrMoV), (Kussmaul (1989)), and on the recently developed Grade 91 steel (9CrMoVNB), (Middleton & Metcalfe (1990)). All demonstrate a susceptibility to Type IV cracking but the actual loss of cross weld rupture strength is variable and unpredictable varying from heat to heat within a given specification and also from one type of steel to another.

Typical data for ⅔CrMoV steel indicates that failures in the Type IV zone in this case occur ~25% below the parent material strength. The loss in strength in other cases is reported to range from the lower bound rupture strength for a particular material, to values as low as 30-40% below the mean parent metal strength, corresponding to a shortfall in time to failure by up to an order of magnitude. Such variations clearly provide significant problems for operators when attempting to assess the operating lives of welds in service. These are accentuated by the actual mechanism of Type IV cracks which initiate and grow within concentrated areas of creep cavitation damage formed within the discrete Type IV region of the HAZ. The cavities themselves are below the limit of resolution for conventional Non-Destructive Examination (NDE), methods, and there is a danger therefore that a weld in an advanced state of cavity damage can be declared defect free and returned to service. Microscopic cracks can then accelerate and grow to macroscopic dimensions in pre-damaged material extremely rapidly with clear implications to plant integrity particularly as the development to macroscopic crack sizes can occur in times well within the statutory inspection times for operating plant.

3.2.4 Project B: Life Assessment of Ethylene-Furnace Tubes

3.2.4.1 Background.

Ethylene furnace tubes operate under the most arduous conditions present in any petrochemical process. A complex combination of factors has an effect on tube life. This has delayed development of a rigorous and successful method of tube-life prediction. However, recent developments at ERA in the life assessment of fired heater tubes in other applications (e.g. catalytic reformers, coker heaters, steam reformers) mean that the development of a mechanistically based model for life prediction of ethylene tubes is now possible. Figure 4 shows a picture of an ethylene plant in Italy.
3.2.4.2 Industrial requirement.

Ethylene furnace tubes operate under the most arduous conditions present in any petrochemical process. In order to crack the hydrocarbon chain, the feedstock and steam have to be heated to approximately 1500°F (800°C) in a fraction of a second and then quenched to avoid excessive carbon formation. To achieve the necessary heating rate, long tube passes are required and heated on the outside to 1900°F (1050°C) or higher. With time, carbon depositions on the tube inner surface necessitates a higher firing rate, and, hence, higher tube wall outer temperature, to compensate for the insulating effect of the carbon deposits. Further, this causes carburization of the tube material to accelerate. A result of this continual process is that the tube wall temperature becomes too high for safe long-term operation or the pressure drop along the coil is excessive. Consequently, the carbon must be removed by a decoking procedure, which can contribute to carburization. Tube failure can occur as a result of ‘hot-spotting’ where carbon build-up or local temperature variations result in escalating carburization and temperature increases. The ultimate life of a given tube coil is frequently governed by the inability, due to carburization of the tube material, to successfully either: (a) weld-in replacement lengths of tube which are required to account for rupture of the original tube due to an upset event
(i.e. a transient); or (b), weld the existing tube after removal of excessively stretched (crept) material.

3.2.4.3 Current Methods of Tube-Life Assessment.

A complex combination of factors are considered likely to have an effect on tube life. As a result of this complexity, development of a rigorous and successful method of tube-life prediction has not been possible. Most operators try to avoid failures during planned run campaigns by using a variety of empirical/service experience tube-management procedures. These may involve a non-destructive assessment of the degree of carburization by monitoring the change in ferromagnetism with a magnetometer or by means of a similar instrument. In addition, gross changes in tube dimensions (length, diameter, bulging etc.) are monitored to assess service creep.

Existing methodologies for life assessment involve manual calculation of the main life-limiting parameters in a simple deterministic manner using approaches similar to those in the original design procedure. As a consequence, life assessments tend to suffer from the same conservatism as design lives. The use of a worst-case scenario (e.g. maximum temperature, maximum stress, minimum wall thickness and materials properties values) of the life-limiting parameters allows the determination of only a very conservative, deterministic, lower bound remaining life. This is of little practical value for cost-beneficial life optimization.
3.3 Creep failure.

In this section the process of deformation and fracture that occur at high temperatures is discussed. The nature of creep and the influence of microstructure, stress and temperature on the modes of deformation and failure are included. The purpose here is to put the diffusive growth mechanism into perspective in terms of the larger scheme of creep failure.

The most general shape of creep curve that is observed is shown in Figure 5. This figure ignores the instantaneous elastic and any plastic strain that take place on loading. Creep in polycrystalline materials occurs as a result of the motion of dislocations within grains, grain boundary sliding and diffusion processes (Cadek, (1988), Riedel (1987)). Webster and Ainsworth (1994), cite further references and the reader is directed to them for more detail. A creep curve can be split up into sections. All of the stages of creep are not necessarily exhibited by a particular material for given testing conditions.

![Figure 5. General form of creep curves, Webster and Ainsworth, (1994).](image)

In Figure 5 the following regions are shown:

**OA** - A region of accelerating creep rate which occurs immediately after the full load has been applied. It is called the incubation period because it happens prior to the attainment of primary, secondary and tertiary creep. It is usually only observed in single crystal or highly oriented materials at relatively low stresses and high temperatures.
**AB** - The primary creep stage. It is a period of decreasing creep rate where work-hardening processes dominate and cause dislocation motion to be inhibited.

**BC** - The secondary or steady-state region of creep deformation. This stage usually dominates the creep life of the material and results in a constant creep rate where there is a balance between work-hardening and thermally activated recovery (softening) processes.

**CD** - The final stage is called the tertiary region. This is a period of accelerating creep rate that culminates in fracture. This can be caused by a number of factors that include; increase in stress in a constant load test, formation of a neck and voiding and/or cracking.

All stages of creep are accelerated with an increase in stress and/or temperature. For most engineering materials plastic deformation occurs more readily than creep at room temperature, whereas at temperatures approximately greater than half the melting temperature of the material the reverse is true. This explains why room temperature design philosophies are based on avoiding yielding and high temperature design codes on avoiding creep failure.

Creep in polycrystalline materials is sensitive to grain size, alloying additions, initial condition of the material, heat treatment and testing conditions. Improvements in creep strength can be achieved by alloying additions to steel. Nickel based superalloys are employed in the highest temperature applications because they exhibit high creep strength at relatively high fractions of their homologous temperatures.

There are several microscopic processes that contribute to creep deformation in metallic materials. The region in which an individual process dominates can be obtained from a deformation mechanism map (Frost and Ashby, 1982). A deformation mechanism map is a plot of normalized stress, $\sigma/E$, where $E$ is Young’s modulus against normalized temperature $T/T_m$. 
Figure 6. Deformation mechanism map for pure nickel with a grain size of 0.1mm, Frost and Ashby, (1982).

Figure 6 shows an example of a deformation mechanism map for pure nickel. It includes lines of constant strain rate and can be used to establish the process controlling creep at a given temperature. For a given mechanism, actual creep rates are dependent on material composition, microstructure and grain size.
3.4 Cavity nucleation models.

3.4.1 Introduction.

Since the pioneering work in the early fifties on intergranular creep cavitation, considerable effort has been made to understand the mechanisms of cavity nucleation and growth in creep. The question of how and where a cavity nucleates is a complex one and, as a result there has been a vast amount of research carried out in this area. In relatively pure metals, there are a number of places cavities may nucleate, these include: intersections of slip bands with grain boundaries possibly due to the stress concentration that occurs here, also at ledges in grain boundaries and on triple grain junctions. Most structural alloys contain second phase particles that are found on the grain boundary, these particles are often preferred cavity nucleation sites. The influence of grain boundary sliding (gbs) has also been discussed at length in the past and it has been shown to concentrate stress on triple grain junctions and on ledges in the grain boundaries. Hence cavity nucleation at these stress concentrations has often been postulated.

The importance of gbs for cavity nucleation was convincingly demonstrated by Chen and Machlin (1957) and Intrater and Machlin (1959). They found that copper bi-crystals develop no cavities under pure tension, but exhibit profuse cavitation if the grain boundary is sheared prior to tensile loading. However, Raj (1975) and Ghandi and Raj (1982) observe cavitation at particles on bi-crystal boundaries under pure tension. Chen and Argon (1981) and Chen and Weertman (1984) demonstrated that cavities are preferentially found on boundaries that are normal to the tensile stress and therefore slide the least. This is contrary to the observations on copper bi-crystals and shows that gbs is not essential for cavity nucleation in polycrystalline materials, (Riedel, 1993).

From the literature there appear to be two approaches to cavity nucleation, theoretical and empirical. These have been treated separately in the following sections.

3.4.2 Theoretical nucleation models.

One approach for modelling cavity nucleation uses the so called classical theory of nucleation where it is assumed that cavity nucleation involves the clustering of vacancies on interfaces subjected to high tensile stresses. There are two main types of nucleation
model; athermal and thermal. These two types have also been the source of much published material and are responsible for the processes of instantaneous nucleation and continuous nucleation respectively. Athermal nucleation processes are those for which the value of the concentrated stress exceeds the critical value of the local cohesive strength, in this process thermal activation plays no role except in reducing the level of stress concentration. From this, it is postulated that, in single phase materials, nucleation should occur instantaneously early in life, (Evans 1984). This was the basis of the Hull and Rimmer (1959) paper, in which they assumed that all the cavities were present at time \( t = 0 \) or are nucleated instantaneously when the load is applied. This precludes the idea of continuous nucleation throughout the lifetime of the material. Thermal nucleation processes are those in which there is a thermally activated condensation of atomic vacancies on the grain boundaries which eventually leads to stable cavities. Nucleation would then occur, not instantly, but in an interval of time determined by the quantity of energy required. In principle this effect could then lead to continuous nucleation of cavities (Evans 1984). Raj and Ashby (1975) and Raj (1979) have explored this process in considerable detail, although mainly for nucleation at particles where the geometry of the embryonic cavity in relation to the particle/matrix interface can be complex but the energy requirements can be reduced. Using the cases of Raj and Ashby (1975) and Raj (1979) where the cavity was assumed to nucleate without the aid of gbs so that the thermal activation was required to attain the stable radius \( R_c \) with an associated energy requirement \( \Delta G_c \), so that

\[
R_c = \frac{2\gamma_s}{\sigma_{\infty}}
\]  

(3.4-1)

This is the size of the critical stable nucleus for which continued growth is energetically possible at the applied stress \( \sigma_{\infty} \). If \( n_r \) is the maximum, fixed number of potential nucleation sites per unit area of grain boundary and \( \Delta G_c \) is the free enthalpy associated with the formation of cavity embryos, then the number \( n_c \) of critical nuclei per unit area is:

\[
n_c = n_r \exp\left( -\frac{\Delta G_c}{kT} \right)
\]

(3.4-2)

Where \( \Delta G_c \) is given by
\[ \Delta G_e = \frac{16\pi\gamma^3}{3\sigma^2} \]  

(3.4-3)

The number of cavity nuclei larger than the critical size formed per second is equal to the product of the number of critical size, \( n_c \), and the probability, \( p_r \), of adding one vacancy to the critical nucleus. This probability is the product of the number of peripheral sites, 

\[ \left( \frac{2\pi R_c Z \Omega_A^{1/3}}{\Omega_A} \right) \exp \left( \frac{\sigma_n \Omega_A}{kT} \right) \]

and the probability

\[ \frac{D_{gb}}{\Omega_A^{2/3}} \]

that one jumps away from the cavity, where \( R_c = 2\gamma_s / \sigma_n \) and the exponential term allows for the increase in vacancy concentration by the local stress, \( \sigma_n \). Thus,

\[ p_r = \left( \frac{4\pi\gamma_s ZD_{gb}}{\sigma_n \Omega_A^{1/3} \Omega_A} \right) \exp \left( \frac{\sigma_n \Omega_A}{kT} \right) \]  

(3.4-4)

Where \( Z \) is the Zeldovich factor, \( D_{gb} \) is the self-diffusion coefficient in the grain boundary and \( \Omega_A \) is the atomic volume. This derivation follows that of Raj and Ashby (1975) except for the subtle difference of replacing the applied stress \( \sigma_w \) in the definition of the critical radius by the local stress \( \sigma_n \). The steady state nucleation rate is given as:

\[ \dot{n} = \left( \frac{4\pi\gamma_s}{\sigma_n \Omega_A} \right) \left( \frac{ZD_{gb}}{\Omega_A^{1/3}} \right) \rho_{\text{max}} \exp \left( \frac{16\pi\gamma^3}{3\sigma^2 kT} \right) \]  

(3.4-5)

Where \( \exp \left( \frac{\sigma_n \Omega_A}{kT} \right) \) has been taken as unity, Evans (1984).

It has been shown that the cavity nucleation rate is small below, and becomes very large above, a certain nucleation stress, which is given by

\[ \sigma_{nc} = \left( \frac{\gamma_s f \nu}{10kT} \right)^{1/2} \]  

(3.4-6)
Here the non-dimensional factor $f_r$ accounts for the cavity nucleus shape, (in the above example it is assumed that the cavity is spherical and has the value of $4\pi/3$). It is defined as cavity volume divided by the cube of the radius of surface curvature. As an example, if the surface energy is taken as $\gamma_s = 1.5 \text{ J/m}^2$ and $T = 850 \text{ K}$, equation (3.4-6) simplifies to $\sigma_{nuc} = 5360\sqrt{f_r} \text{ MPa}$. This shows that the predicted nucleation stress is too high compared to observed values, unless the volumetric function $f_r$ is of the order $10^{-5}$ to $10^{-4}$. Riedel (1993) states that it is not likely that cavity nuclei generally have the extreme shapes corresponding to such small values of $f_r$. An example of a theoretical nucleation model is shown in Figure 7, where the cavity nucleation rate in copper is shown as a function of tensile stress for three values of $f_r$, (Raj 1975). The striking feature is the strong dependence of nucleation rate on $f_r$ and particularly, on local tensile stress which is the driving force for nucleation, thus giving the appearance of a “threshold stress” below which the nucleation rate is virtually zero. It can be seen from the figure that this “threshold stress” is unrealistically high unless the shape factor $f_r$ is very low, (in the region of $10^{-4}$), thus agreeing with Riedel (1993).

![Figure 7. Graph showing steady state nucleation rate as a function of tensile stress in Copper at 923 K from Raj (1975).](image)

- $f_r = 10^{-5}$
- $f_r = 10^{-2}$
- $f_r = 0.5$

x = "Threshold Stress"
Applying the classical nucleation theory leads to predictions of stresses which are found to be 30-300 times greater than the applied stresses at which nucleation still occurs (Argon 1982). Due to these inconsistencies it has been discussed (e.g., Argon (1983), Goods and Nieh (1983), Riedel (1984, 1987)) whether the stress could be raised locally to the required levels by stress concentrations at slip bands or due to gbs. Dyson (1983) concludes that because of the stochastic nature of the polycrystal matrix deformation, cavity nucleation is continuous and related to strain, in accordance with numerous observations. Grain boundary sliding does not play any significant role according to the model. Svoboda and Sklenicka (1990), argue that the stress concentrations at intergranular inclusions caused by gbs need not influence the cavity nucleation rate significantly, though the stress concentrations are higher than those originated in other mechanisms. Riedel (1993) states that as a result of the stress analyses it appears that the stress concentrations cannot be exceedingly large, and are hardly sufficient to reach the theoretical nucleation stresses. Thus the problem of cavity nucleation cannot be regarded as being quantitatively understood. Svoboda (1993) studied the co-operation of surface diffusion of matrix atoms to the cavity/grain boundary junction and the diffusive transport via the grain boundary where they are deposited. This was accomplished using the variational principle and the equations specified the Gibbs free energy of the cavity $G$ as being a function of the number of matrix atoms, $n_1$, and the number of inclusion atoms, $n_2$, removed from the cavity. The author states that due to the stochastic nature of the cavity evolution in the $(n_1, n_2)$ space, the concept of a nucleation barrier and critical cavity state is failing and these terms ceased to be well defined. Shewmon and Anderson (1998) state that the process of gbs gives no satisfactory explanation for the development of a uniform array of voids on boundaries normal to the applied stress.

3.4.3 Empirical nucleation models.

Numerous experimental investigations arrive at the common conclusion that cavity nucleation starts early and is continuous and approximately linear with the time dependant strain and increases with the applied tensile stress over the entire creep life (Needham and Gladman, 1980; Dyson, 1983; Wilkinson, 1986 and Davanas & Solomon, 1990;). Needham and Gladman (1980), suggest that for creep of type 347 stainless steel:
\[ n_{\text{cov}} = B \varepsilon, \]

Where \( n_{\text{cov}} \) = number of cavities nucleated per unit grain boundary area, \( B \) = nucleation constant which depends on the material (m\(^2\)) and \( \varepsilon \) = time dependant global creep strain. Differentiating the above equation with respect to time \( (t) \), assuming \( B \) = constant, yields:

\[ \dot{n} = B \dot{\varepsilon} \quad (3.4-7) \]

Where \( \dot{n} \) = rate of nucleation (per unit area and time), of cylindrical cavities of critical radius, \( R_c = \gamma_s \sin \Psi / \sigma \) (\( \Psi \) = dihedral angle) and \( \dot{\varepsilon} \) = time dependant creep strain rate (s\(^{-1}\)). This shows that the nucleation rate is proportional to the strain rate. Dyson (1993) states that the factor of proportionality \( B \) varies greatly from material to material. It ranges from \( B = 10^9 /m^2 \) or less for high purity steels, over \( 4 \times 10^{10} /m^2 \) for a commercial steel quality to \( 4 \times 10^{12} /m^2 \) for a coarse-grained heat affected zone material which contains finely dispersed sulphides on its grain boundaries. The corresponding creep ductilities vary between 20\% and 2\% strain to rupture. Davanas and Solomon (1990) used a trial and error technique to match the predicted time with the measured rupture time for copper at 5 MPa and 1023K. Using the Monkman-Grant constant (Evans, 1984) of 0.06, and the appropriate steady state creep rate, \( \dot{\varepsilon}_s \), for these conditions yields a rupture time of \( 7.84 \times 10^5 \)s, from this they arrived at the value of \( B = 1.6 \times 10^7 m^{-2} \). They assumed that the value of the nucleation rate constant, \( B \), was stress and temperature independent. The value of \( B \) was determined by calculating how long it would take for the grain boundary to become 85\% cavitated using the nucleation model as well as ripening and interconnection of existing cavities. Dyson (1983) and Riedel (1987) compile experimental evidence for the approximate validity of equation (3.4-7) and also quote results that deviate from that expression. The possibility of a critical stress required for cavity nucleation is discussed. For ferritic steels such a critical stress certainly lies below the usual design stresses (50 to 100 MPa), since many of them develop cavities during service. In pure metals, cavity nucleation is still observed at stresses below 10 MPa. The most important results from the above papers can be summarized as follows:

a) no incubation time for cavity nucleation was observed;

b) at small creep strains (up to about 0.05), the number of cavities, \( N_A \), increased linearly with strain;
c) nucleation was either continuous until fracture intervened or cavity saturation occurred;
d) strain was the parameter controlling the number of cavities and not time;
e) the rate of cavity accumulation varied greatly from material to material (the higher the rate the lower the ductility and vice-versa), (Dyson, 1983).

As a means of comparison, Figure 8 shows a selection of the nucleation rates from some of the reviewed nucleation models whose expressions are given below the figure.

![Figure 8. Comparison of different nucleation models for copper at 1023 K.](image)

\[
\dot{N} = \frac{4\pi \gamma_s}{\sigma_n \Omega^{4/3}} D_b \delta \rho \times \exp \left( -\frac{4\gamma_s^2 f(\alpha)}{\sigma_n^2 kT} \right) - \text{Raj}
\]

\[
\dot{N} = Z \left[ \frac{4\pi \gamma_s}{\sigma_n \Omega^{4/3}} \right] D_b \delta \rho \times \exp \left[ -\frac{4\gamma_s f(\alpha)}{\sigma_n^2 kT} \right] - \text{Shewmon and Anderson}
\]

The above models are the two theoretical based nucleation models. Where \( f(\alpha) \) accounts for the cavity nucleus shape, \( \rho \) gives the total number of nucleation sites per unit area, \( \delta \) is the boundary thickness and \( Z \) is the Zeldovich factor.
Here, the above two models are the empirical based nucleation based models. Where $D_v$ is the lattice diffusion coefficient, $B$ and $A$ are material constants, $b$ is the burgers vector and $n$ is the creep exponent.

The main purpose of this is to demonstrate how the different models predict nucleation under approximately the same conditions. It can be seen from the figure that there are large differences in the way the models predict nucleation. The models based on the classical nucleation theory by Raj (1975) and Shewmon and Anderson (1998), clearly show the presence of a “threshold stress” which corresponds to a non-dimensioned nucleation rate of unity. This ‘threshold stress’ can be seen to be much higher than the minimum stress value that has been observed by experiment to cause nucleation. The two empirical based models by Davanas and Solomon (1990) and van der Giessen & Tvergaard (1994), are linear in nature and show nucleation occurring at much lower stresses but continuing to increase rather than reaching a maximum rate. It should also be noted that due to the fact that no numerical values were given for the material constants in the van der Giessen model, this author adjusted values from Davanas and Solomon (1990), and used them as an alternative.

It has been shown in this section that there is widespread opinion as to how the process of nucleation takes place. The classical based nucleation theory predicts nucleation only to occur above a ‘threshold stress’, which tends to be significantly higher than the stress nucleation is observed to occur at by experiment. For this reason it has been decided that this work will use an empirical based model such as the one used by Davanas and Solomon.
3.5  Cavity growth models.

3.5.1  Introduction.

After the initial nucleation of cavity nuclei, and once they have reached the critical size, they can grow under creep conditions and develop into large cavities which are easily observable by light microscopy (Shown in Figure 9).

![Figure 9. An example of intergranular cavitation in silver when annealed in oxygen and hydrogen each for two hours at 900°C. Goods & Nix, (1977).](image)

The growth of intergranular cavities occurs by the absorption of vacancies by cavity surfaces. This can be controlled by solid state diffusion, by coupled solid state diffusion and plastic flow or by plastic flow alone. As shown in Figure 11, the complete process of intergranular cavity growth involves grain boundary diffusion, surface diffusion, power-law creep and grain boundary sliding. The size and shape of cavities changes with time and is different from one grain boundary to another due to non-uniform and continuous nucleation of new cavities. Also the position and boundary conditions are different for each grain boundary, making a large number of growth conditions possible. This makes the process of cavity growth a complex one and there have been many mechanisms of growth considered for various temperatures and stress conditions.

Dyson, (1979) first investigated the effects of constrained cavity growth. There are two limiting modes of cavity growth that occur under creep conditions (Nix, 1983): (a) unconstrained cavity growth and (b) constrained cavity growth. In the case of unconstrained cavity growth, cavities are present on all the grain boundaries in the
polycrystal and are free to grow up to the point of complete failure. In the case of constrained cavity growth, cavities are present only on isolated boundaries. Here cavity growth on the cavitated boundary can proceed only if the surrounding continuum creeps. This is due to the fact that the relative grain displacements associated with the cavitation have to be accommodated by corresponding displacements in the matrix. Consequently cavity growth may be limited entirely by creep flow of the matrix (Nix, 1983).

Three of the main mechanisms which control the growth of cavities are shown in Figure 10 (Cocks and Ashby, 1982). These are:

1. When grain boundary diffusion is slow void growth is controlled by boundary diffusion; matter diffuses by boundary diffusion out of the growing void and plates on to the grain boundary. Here, the void remains spherical because surface diffusion rapidly redistributes matter within it (Figure 10a).

2. Void growth controlled by surface diffusion. When surface diffusion within the void is slow, it ceases to grow like a sphere. Matter flows out of it at the equator, causing it to become flatter and more crack-like (Figure 10b) until the curvature difference between the poles and the equator is sufficient to drive a surface flux which matches that leaving, by boundary diffusion at the equator.

3. Void growth by power-law creep. When the void grows by the power law creep of the surrounding matrix. In simple tension the shaded slab containing the void in Figure 10c extends at a rate determined by the net section stress, while the

Figure 10. Three mechanisms that limit void growth: a) Boundary diffusion, b) Surface diffusion, and c) Power-Law creep. (Cocks and Ashby, 1982).
rest of the cylinder (unshaded) extends at a rate determined by $\sigma_c$ (equivalent tensile stress).

Figure 11 shows an example of a mechanism map of creep cavity growth for pure copper. It can be used to establish the process controlling creep at a given stress and temperature.

![Figure 11. A void growth map for copper (Cocks and Ashby, 1982).](image)

The void growth mechanism map shows two main fields. In one, the void growth rate is governed by the glide and climb of dislocations and has a power law stress dependence. In the other, void growth is controlled by the stress directed diffusional flow of atoms.

It can be seen from Figure 11 that for a low applied stress the growth rate is controlled by boundary diffusion for the whole range of operating temperatures. Whereas for higher applied stresses with temperatures less than $0.5T_m$ the growth rate is controlled by surface diffusion. If the temperature is increased for this stress range the controlling mechanism changes to power-law creep. If the operating stress is raised even higher the growth rate is controlled by plastic deformation.
This work is centred on the region in which the creep damage is controlled by coupled surface and grain boundary diffusion. We therefore look at temperatures up to approximately 0.6T_m with stresses in the range of $10^{-3} \sim 10^6 \sigma / E$.

These processes will be looked at in detail in the following review of published work on cavity growth, with a view to highlighting the effects of each of the mechanisms in the models. The different processes of cavity growth are much better understood than the processes of cavity nucleation. Riedel (1993), states that comparisons with experiments suggest that for structural alloys tested under low-stress, long-time conditions, the constrained diffusive mechanism is the most important one. However, it has also been shown that unconstrained growth is important when looking at bi-crystals and should not be overlooked as a growth mechanism.

3.5.2 Diffusional growth models.

Diffusional growth models assume that growth occurs by absorption of vacancies by cavities. Vacancies are generated at grain boundaries and diffuse to cavities through the boundaries, while atoms from the cavity surfaces are deposited on the boundaries. A difference in chemical potential of a vacancy in a boundary that is acted on by a tensile stress $\sigma_n$ and the potential of a vacancy at the cavity surface, causes vacancy diffusion. If the cavity radius is greater than $R_c$ in equation (3.4-1), the chemical potential of a vacancy on the boundary is greater than that at the cavity surface. Therefore, flow of vacancies from the boundary to the cavity takes place.

Hull and Rimmer (1959), performed the first detailed analysis of diffusive cavity growth, their work was based on the following assumptions:

a) the surface diffusion is sufficiently fast so that the cavity remains spherical;

b) the grains behave as rigid ‘blocks’;

c) the grain boundary diffusion is much faster than lattice diffusion;

d) the grain boundary is a perfect source for vacancies and maintains an ‘equilibrium’ between vacancy concentration and normal stress;

e) the normal stress at the cavity tip with radius ‘a’ has the value $2\gamma_r / a$;
f) a movement of the grains in a direction normal to the boundary is not constrained by external factors.

Hull and Rimmer (1959) also assumed that the cavities are arranged on a square grid in a grain boundary plane. An improvement to this was later suggested by Raj and Ashby (1975), where they considered a circular arrangement of cavities. This was an approximation, but it simplified the mathematics and made the solution more manageable. They also assumed that the cavities were uniformly spaced a distance of $2b$ apart. Raj and Ashby started from Herring's, (1950), relation for vacancy flux

$$J_{gb} = -\frac{D_{gb} \nabla \mu}{kT\Omega_A}$$

where $\nabla \mu$ is the gradient of the chemical potential. On the surface of a cavity of radius $a$, the chemical potential is $\mu = -\frac{2\gamma_s \Omega_A}{a}$, and on the grain boundary the chemical potential is $\mu = -\sigma_n \Omega_A$. The gradient $\nabla \mu$ is given by (3.5-1).

$$\nabla \mu = -\frac{\Omega_A}{b} \left(\sigma_n - \frac{2\gamma_s}{a}\right)$$  \hspace{1cm} (3.5-1)

giving

$$J_{gb} = \frac{D_{gb}}{kTb} \left(\sigma_n - \frac{2\gamma_s}{a}\right)$$  \hspace{1cm} (3.5-2)

Where $b$ is the half cavity spacing. Assuming that diffusion takes place through the area $2\pi \delta_{gb} a$ and the cavity remains spherical during the growth, the rate of increase in cavity volume is given by

$$\frac{dv}{dt} = \dot{v} = \frac{2\pi D_{gb} \delta_{gb} a}{kTb} \left(\sigma_n - \frac{2\gamma_s}{a}\right)$$  \hspace{1cm} (3.5-3)

From equation (3.5-3) it can be seen that for spacings where $2b \gg a$, the volumetric growth rate will be very slow. It should be noted that (3.5-3) is not a precise model.
Speight and Beere (1975), state that the volumetric growth of cavities occurs by two interrelated processes. The first is the absorption of all the vacancies generated on the grain boundary area at the cavity. This is expressed as

\[ \left( \frac{dv}{dt} \right)_A = \pi \beta \Omega_A (b^2 - a^2) \]  

(3.5-4)

Where \( \beta \) is the rate of vacancy creation per unit boundary area. Atoms deposited at the grain boundary causes displacement of the grains separated by the boundary in a direction normal to boundary plane at the rate \( \beta \Omega_A \), which is referred to as the 'jacking' rate, and is defined as

\[ \left( \frac{dv}{dt} \right)_B = \pi \beta \Omega_A a^2 \]  

(3.5-5)

The 'jacking' component becomes important when the cavity has grown to such a size that its diameter is comparable to the cavity spacing. The total volumetric growth rate is given by summing equations (3.5-4) and (3.5-5), and is given by

\[ \frac{dv}{dt} = \pi \beta \Omega_A b^2 \]  

(3.5-6)

Speight and Beere (1975) derived the expression for rate \( \beta \), and substituting it into equation (3.5-6) they obtained the following expression for volumetric cavity growth rate

\[ \frac{dv}{dt} = \frac{8 \pi \Omega_A D_g \delta_{gb} \sigma}{kT \left[ 4 \ln \left( \frac{b}{a} \right) - \left( 1 - \left( \frac{a}{b} \right)^2 \right) \left[ 3 - \left( \frac{a}{b} \right)^2 \right] \right]} \]  

(3.5-7)

Raj and Ashby (1975) derived a similar equation that does not include the contribution given by equation (3.5-3), these authors did not take into account the effect of 'jacking' i.e. that cavities are forced open when atoms are deposited on the adjoining grain boundary. Davanas and Solomon (1990) also used a similar growth model and assumed quasi-equilibrium growth that took 'jacking' into account, as well as cavity growth and interconnection. For uniform cavity sizes and spacings, the equations reduce to
where $a$ is cavity radius, $\theta$ is dihedral angle and $b$ is cavity spacing. It is quoted by the authors as being equivalent to Chuang et al., (1979). It should be noted that (3.5-7) is a 3 dimensional model, whereas (3.5-8) is 2 dimensional.

For a spherical cap cavity of radius $a$, it holds that

$$\frac{dv}{dt} = 4\pi a^2 \frac{da}{dt} h(\Psi)$$

(3.5-9)

where

$$h(\Psi) = \left[ \frac{1}{1 + \cos \Psi} - \frac{\cos \Psi}{2} \right] / \sin \Psi$$

(3.5-10)

and is used to define the shape of the cavity using the half dihedral angle ($\Psi$). For the special case of $b = 5a$ and $\Psi = 70^\circ$, equation (3.5-7) reduces to

$$\frac{da}{dt} = \dot{a} = \frac{D_{gb} \sigma \Omega}{kT a^2}$$

(3.5-11)

This shows that the equilibrium cavity growth rate increases linearly with stress. Equation (3.5-8) also reduces to a form similar to that in (3.5-11) above.

Figure 12. (a) Quasi-equilibrium grain boundary cavity. (b) Non-equilibrium (crack-like) cavity. $\Psi$ denotes the angle between the tangent to the cavity at the cavity tip and the x-axis (half dihedral angle), Chuang et al. (1973).
All the models discussed have assumed that the grain boundary diffusion is much faster than the surface diffusion and, because of this, the cavity maintains a spherical-cap shape during its evolution (Figure 12).

However, if the surface diffusion is slower than the grain boundary diffusion the cavity evolves into a narrow crack-like shape. Chuang and Rice (1973) presented the first analysis of the growth of cavities by surface diffusion, however they assumed steady state conditions and did not solve the complete problem. The solution they presented did not include applied stress and was in terms of crack velocity \( v \). This work was extended by Chuang et al., (1979) and Martinez and Nix (1982), who derived expressions for cavity growth rate as a function of stress. In this earlier paper they consider the growth of pre-existing voids along a planar grain boundary for two cases: (i) a long cylindrical void, and (ii) an axisymmetric void. No nucleation of cavities has been included as in the Hull-Rimmer model. The assumption is also made that the slope of the void everywhere is small with respect to unity (an assumption that is violated in most metals), this linearizes the governing equations. For quasi-equilibrium growth controlled by grain boundary diffusion they obtained the equation

\[
v = \frac{3\Omega A D_{gb} \delta_{gb}}{2d(1-d^2)^{\frac{3}{2}}} Q kT b^4 h(\Psi) \left[ \sigma_\infty - 2 \frac{1-d^2}{d} \frac{\gamma_s \sin \Psi}{b} \right]
\]

(3.5-12)

For non-equilibrium growth of a crack-like cavity, the authors derived the equation

\[
v = \frac{27 D_s \delta_s \Omega A}{8 kT(2b)^3} \frac{(1 + Q \Sigma \Delta)^{\frac{3}{2}} - 1}{Q^3(1-d^2)^{\frac{3}{2}}}
\]

(3.5-13)

Where \( \Delta = D_s \delta_s / D_{gb} \delta_{gb} \) (\( \delta_s \) is the thickness of the surface layer through which surface diffusion occurs, \( d = a/b \) and \( \Sigma = 4\sigma_\infty b / [3\gamma_s \sin(\Psi/2)] \). The reader is directed to the paper for the expression for \( Q \) where it can be found in full.

From the analysis of the available \( D_{gb} \) and \( D_s \) data it can be seen that, usually \( \Delta > 1 \). Chuang et al., (1979), state that, in this case that the quasi-equilibrium mode is favoured. This is also the case when the stress level is low and when the cavity diameter and ratio of
diameter to spacing is small. The crack like mode is favoured at high stresses, larger diameters and small ratios of $\Delta$. The model used by the authors is shown in Figure 13.

![Figure 13: Semi-analytical model for cavity system, Chuang et al., 1973.](image)

In order to investigate the transition from the surface diffusion controlled extreme to the grain boundary diffusion controlled one it is necessary to allow the cavity to be able to be both crack-like and rounded. This has been done by Martinez and Nix (1982) using finite difference techniques to solve the diffusion equation on the cavity surface and using steady state solutions for diffusion in the grain boundary. The initial cavity surface is discretized by a set of $N+1$ equally spaced points. The curvature is calculated at each of these points and then using these values, the normal velocity is calculated. The evolution of the free surface is simulated with greater accuracy than by using an arc. The authors found that the number of initial points was a key factor in the stability of the method. Acceptable results were obtained if the initial number of points was between 5 and 11. If this number exceeded 20 the numerical calculations become unstable after a few iterations.

Recently Cocks (2000), has demonstrated modelling void evolution by surface diffusion using an ellipse to represent the cavity. Another method suggested was to model void evolution by combined surface and grain boundary diffusion using a rectangle to represent the cavity. The accuracy of these models remains to be investigated, and can be obtained by comparison with a full finite element solution.
3.5.3 Coupled diffusion and Power-Law growth models.

In purely diffusive cavity growth models it is assumed that the grains behave as rigid blocks and do not deform plastically. It is also assumed that the separation of the grains occurs uniformly across the entire length of the uncavitated grain boundary. It has been shown that the grains deform by dislocation creep above normalized stresses of $\sigma_\infty / E = 10^{-4}$ and temperatures of $0.4T_{\text{melt}}$. The problem of cavity growth by coupled diffusion and power-law creep has been studied by Beere & Speight, (1978) and later by Svoboda and Čadek (1987). Beere and Speight presented a simplified version in which the grain boundary occupied by a cavity is divided into two regions (Figure 14).

![Figure 14. A cavity of radius $a$ is associated with an area of grain boundary of radius $c$. Vacancies created in Region I, radius $b$, diffuse to the cavity. Beere and Speight, (1978).](image)

In Region I, vacancies are generated uniformly in the boundary and diffuse into the cavity. An opposite flow of atoms, which are deposited on the boundary in Region I wedges the boundary apart. In Region II, no vacancies are created, but the displacement in Region I caused by the wedge of atoms is accommodated by power-law creep.

Figure 14 shows a plan view of a cavity on a grain boundary, and the different regions associated with the growth mechanisms. This is a simplification of the square unit cell assumed by Hull and Rimmer, (1959). Figure 15 shows a more detailed picture of how the regions are related to the overall layout of a grain boundary with a number of cavities growing on it. Here, Cocks and Ashby, (1982), isolate a cylindrical element of material of
diameter $2l$ (the void spacing) and height $d$ (the grain size), centered on a grain boundary void of radius $2r_v$. This figure does not show the different regions as defined in Figure 14, but is used to demonstrate where the regions are found.

![Figure 15. Void growth on a grain boundary, showing the Unit of structure. Cocks and Ashby, (1982).](image)

As a result of the regions defined in Figure 14 a distribution of stress occurs across the boundary (Figure 16). In the limiting case of very low applied stresses, Region II is very small so that $c$ tends to $b$. The rate of cavity growth is then entirely controlled by diffusion and is described by (3.5-7).

![Figure 16. Normal stress acting across the grain boundary. Beere and Speight, (1978).](image)

Beere and Speight (1978) obtained the following expression for the tensile stress variation throughout Region I at a distance $r$ from the cavity centre:
\[
\sigma = \frac{2\gamma}{a} + \frac{\left(\sigma_l - \frac{2\gamma_s}{a}\right) \left(2b^2 \ln \frac{r}{a} + a^2 - r^2\right)}{\left(2b^2 \ln \frac{b}{a} - \frac{a^4}{2b^2} + 2a^2 - \frac{3b^2}{2}\right)} \quad (3.5-14)
\]

Where \(\sigma_l\) is the average stress acting over the combined areas of Region I and the cavity.

The tensile stress acting in Region II is equal to the maximum tensile stress acting in Region I, and is found by putting \(r = b\) in equation (3.5-12). The cavity growth rate can be expressed by equation (3.5-6), where \(\beta \Omega_d\) is the jacking velocity due to atom plating on the boundary. The authors used boundary conditions to determine \(\beta\). Using the expression for \(\beta\), the cavity growth rate becomes

\[
v = \frac{2\pi D_b \omega \Omega_d}{kT} \frac{\sigma_l - \frac{2\gamma_s}{a}}{\ln \left(\frac{b}{a}\right) - \frac{1}{4} \left(\frac{a}{c}\right)^4 + \left(\frac{a}{c}\right)^2 - \frac{3}{4}} \quad (3.5-15)
\]

Assuming the relation \(\dot{\varepsilon} = A(\sigma / G)^n\) for Region II and accepting the assumptions made by Beere and Speight (1978), one eventually arrives at three expressions with three unknowns of \(\sigma_l\), \(\sigma_{II}\) and \(b\) which can be solved.

The analysis of Svoboda and Čadek (1987) is similar to that of Beere and Speight (1978). The authors assumed that the cavity growth is unconstrained and the model takes account of all of the important features of contemporary models except grain boundary sliding. They pay particular attention to when power law creep becomes important, and at the same time, assume surface diffusion is much slower than grain boundary diffusion. Thus making it possible to study the evolution of cavity shape during its growth from a spherical-cap (quasi-equilibrium) shape to a crack-like (non-equilibrium) shape. The model employed by Svoboda and Čadek (1987) uses the same boundary conditions as Beere and Speight (1978), and can be solved numerically to give all the required information on cavity growth. The results of the modelling concentrate on axisymmetric cavity shape development during growth from a spherical-cap shape to a non-equilibrium or crack-like shape. Wilkinson (1988), considered the effect on the global rate of void growth of non-uniform distribution of voids on a grain boundary facet. Three controlling void growth mechanisms were considered: grain boundary diffusion, surface diffusion and
power-law creep. In each case the relationship between the global rate of void damage and the nature of the void distribution was considered. Wilkinson, (1988) states that an inhomogeneous void distribution results in a lower global damage accumulation growth rate than that due to a uniform distribution. Up to about a fivefold decrease is predicted for heavily clustered distributions. The stress and temperature dependence for void growth is not affected, as long as coalescence is neglected (i.e. at small cavitated area fraction). A large variation in void growth rate is predicted, with isolated voids growing much faster than those in clusters.

3.5.4 Constrained growth models.

As mentioned in the introduction the second limiting mode of cavity growth is the constrained type. In this case the grains are not able to move apart in an unconstrained manner. In polycrystals subjected to creep the cavities can be distributed uniformly in grain boundaries normal to the tensile stress. It is also found that the number of cavities can vary significantly from one boundary to another.

![Figure 17. Illustration of constrained cavity growth on a grain facet, (Riedel, 1993).](image)

If cavitation is confined to isolated facets which are surrounded by undamaged material then the growth of the cavities is said to be constrained (Figure 17). Dyson, (1976, 1979) assumed that the cavities grow easily under the applied stress by diffusion of atoms away from the cavity and into the grain boundary, and that the surrounding material behaves rigidly. This means that the increased volume of the growing cavities cannot be accommodated, and, as a result the rigid material exerts a back stress on the cavitating
boundary. This means that the local grain boundary stress that is the driving force for the 
diffusion is reduced by ‘load shedding’ from the cavitated grain boundary onto the 
surroundings. This occurs until the normal stress $\sigma_n$ that they carry is sufficiently reduced 
relative to the applied stress $\sigma_\alpha$ that the rate of cavity growth is equal to the rate at which 
the surrounding material can accommodate the increased volume by creep flow. This 
means that if the material is creep-resistant, the cavity growth process is controlled by the 
rate of creep of the material. If the material creeps easily, then the increased volume is 
accommodated easily and the cavity growth rate is controlled by the diffusive growth 
process itself. This is the unconstrained limit (Riedel, 1993).

Constrained cavity growth was first discussed by Dyson (1976, 1979) and later treated by 
Rice, (1981) and was later improved on by several authors (see, e.g., Riedel 1987). Rice, 
(1981), assumed that the cavities were spherical-capped in shape of radius $a$, half dihedral 
angle $\Psi$ and spacing $2b$ (defined in Figure 17). Norton’s power law was assumed to 
describe the surrounding creeping matrix. The normal tensile stress acting on the grain 
boundary facet, $\sigma_n$, and a transverse stress, $\sigma_t$, are applied remote from the facet, and the 
facet transmits a back stress, $\sigma_b$, which is controlled by the rate at which the surrounding 
matrix creeps being compatible with the diffusive growth rate of the cavities. Riedel, 
(1993), states that, under these conditions the cavity growth rate is obtained as

$$
\dot{K} = \frac{\sigma_n - (1 - \omega)\sigma}{h(\Psi)a^2} \frac{q'(\omega)kT}{2\Omega_A D_{gb} \delta_{gb}} + \frac{q'\sigma_e}{\varepsilon_e 4b^2 d}
$$

(3.5-16)

Where $\Omega_A$ is atomic volume, $D_{gb} \delta_{gb}$ is the grain boundary diffusion coefficient (in m$^3$/s), 
$\omega = (a / b)^2$ is the cavitated area fraction of the grain facet, $q' = \pi^2(1 + 3/n)^{1/2}$ is an 
abbreviation, $\sigma_e = |\sigma_n - \sigma_t|$ is the von Mises equivalent stress and $\varepsilon_e$ is the equivalent 
strain rate. The sintering stress is given by

$$
\sigma = \frac{2\gamma_s \sin \Psi}{a}
$$

(3.5-17)

and the dimensionless function, which accounts for the lenticular cavity shape is given by
Equation (3.5-16) contains the limiting cases of constrained and unconstrained cavity growth. It can be seen that if the strain rate is high the second term in the denominator vanishes. The stress on the boundary is then equal to the applied tensile stress and the cavity growth rate is that of unconstrained diffusive growth. If the strain rate is low, the first term in the denominator becomes negligible, and the cavity growth rate is proportional to the strain rate. Riedel, (1993) states that in this case the stress on the boundary is reduced to the sintering stress, a value that is generally small compared to the applied stress. Therefore at the constrained limit the boundary facet acts mechanically like a microcrack which transmits no appreciable tractions. Cocks, (1985) investigated cavity growth constrained by grain boundary particles. The growth of cavities by grain boundary diffusion was analysed with the assumption that grain boundaries are perfect sources and sinks for vacancies. The rate of growth is constrained by the ease with which material can plate out around the particles or the rate at which the material surrounding the particles can deform by power law creep. The author assumed that once the stress at the particle reaches the critical value, it completely detaches itself from the boundary creating a void of radius \( r_p \).

This assumption led to the idea of how cavities are continuously nucleated during creep. It has been found that Power-law creep is favoured at large particles and diffusion at small. As a result, there is a critical particle size, above which accommodation occurs by power-law creep and below which by diffusion. The stress is at a maximum at these particles. Tvergaard, (1984) considered the axisymmetric problem of grain boundary cavitation constrained by creep deformations of the surrounding grains. Grain boundary diffusion was the only diffusive mechanism considered and grain boundary sliding was not accounted for separately. The results presented were based on the assumption that the cavities are present at the initial stage, thus not considering the time required to nucleate cavities. The simplified model produced gives good approximations of solutions produced by finite element method. The author also states that the numerical analyses for non-
uniform initial cavity sizes indicate that the smaller voids will catch up so rapidly that
neglecting the size differences may be a good approximation. However, he also states that
different spacings between cavities are not evened out and it has been shown that more
closely spaced voids on some part of the facet will link up much earlier than predicted
based on the average spacing.
3.6 Diffusional crack growth.

3.6.1 Introduction.

Riedel, (1987), states that creep crack growth is the time-dependent extension of a macroscopic crack at elevated temperatures under more or less constant load. A macroscopic crack, as distinct from grain boundary cavities, is a crack that is larger than the structural lengths of the material that are relevant for crack growth (for example, the grain size). In order to develop models of intergranular creep failure, good understanding of the processes of creep crack growth by intergranular cavitation is very important. Cocks and Ashby, (1983) investigated creep crack growth assuming that the growth of a uniform array of cavities was the rate determining step during creep fracture, but in reality cavities are distributed non-uniformly and grow at different rates. There is usually some coalescence of cavities and facet crack formation that occurs well before final failure.

3.6.2 Numerical models.

There have been many numerical models suggested for the growth of cracks at high temperatures. Beere and Speight, (1978) assumed that the crack propagated continuously due to plastic flow enhanced diffusion, whereas Chuang and Rice, (1973) assumed that it was continuously due to diffusion of vacancies to it’s tip and deposition of atoms on the grain boundary facet. Riedel, (1987) states that observed growth rates can be explained consistently if local failure at the crack tip is assumed to be strain controlled. The agreement is still good if local failure is brought about by stress controlled cavity nucleation and strain controlled growth. The models based on diffusion-controlled cavity growth disagree with the observed creep crack growth behaviour. The case of diffusive growth and strain-controlled nucleation could not be treated because of mathematical difficulties. Riedel, (1987) states that if such a model were available it could explain the measured data.

Wilkinson and Vitek, (1982), formed a general theory regarding crack propagation and it provides a basis which can be used to describe the growth under a variety of different
conditions. The system assumed by the authors is shown in Figure 18a. The crack and cavities are assumed as infinite in the plane parallel to crack surfaces, and it is loaded under tension by a remote stress $\sigma_{\infty}$ normal to the crack. The crack propagates due to growth ahead of its tip. The authors assumed an array of $N$ cavities, spaced at a distance $c$ apart. A steady state form of crack growth occurs when the number of cavities $N$, which grow simultaneously ahead of the crack remains constant as the crack advances. When the cavity nearest the tip grows to a size sufficient for linkage to occur, a new cavity is nucleated at the end of the row. Thus the crack grows in jumps requiring a time interval $\Delta t$.

![Figure 18. (a) A crack (half-length $a$) loaded in tension by remote stress $\sigma_{\infty}$. (b) The $n^{th}$ cavity is loaded by the local stress $\sigma_n$, and grows at a velocity $v_n$ along the grain boundary. Wilkinson and Vitek, (1982).](image)

The authors assumed that the stress at a distance $x$ from the crack tip is $\sigma = (A/x)^\alpha$, where both $A$ and $\alpha$ are positive and $A$ is a function of external loading, crack length and specimen geometry. Thus the $n^{th}$ cavity removed from the crack (shown in Figure 18a), is loaded by a local stress

$$\sigma_n = (A/c_n)^\alpha$$

(3.6-1)

The authors assumed that the cavities growth under the effect of the applied stress takes place by diffusion, plastic flow or a combination of both of these mechanisms. After the time interval $\Delta t$, the cavity nearest the cavity tip has become large enough for linkage with the crack tip to occur. During this time interval each cavity grows from the length it has at the beginning of the time interval, i.e., $2l_n$, to that of its neighbour nearer the crack at the same time, i.e., $2l_{n+1}$, this is shown in Figure 18b. The average crack growth rate by this
process is given by $\dot{a} = c/\Delta t$. The authors considered cavitation by both diffusion and power-law creep. They analysed two cases of diffusion controlled cavitation, the first was for equilibrium shape cavities where surface diffusion was assumed to be much faster than grain boundary diffusion; the second was for a crack-like cavity. The authors found that, in general, crack growth rate depends on the number of cavities, $N$, growing simultaneously ahead of the crack. This number is controlled by the nucleation mechanism, which can vary widely according to the conditions. Thouless et al., (1983), also assumed fast surface diffusion in their model for crack growth in polycrystals. This meant that the cavities on the grain boundary were expected to be of an approximately uniform size. The model considered by the authors consisted of a damage zone ahead of the crack containing an array of grains co-planar with the crack and embedded in a linearly viscous matrix (Figure 19). The growth of cavities was assumed to be constrained by the viscous matrix.

![Figure 19. Theoretical model of Thouless et al. (1983), showing damage zone ahead of crack tip.](image)

Grain boundary sliding between the grains in the damage zone is assumed to accommodate the damage gradient and hence, equalize the stress on each grain. The authors state that the crack extension is macroscopically Mode I and occurs locally on boundaries inclined to the crack surface, this is shown in Figure 20. These boundaries are subject to both shear and normal stresses.
Chuang et al., (1996), investigated the high temperature growth behaviour along a planar interface between two elastic dissimilar media. The authors assumed that the crack grows along the interface normal to a remote applied tensile stress via coupled surface and grain boundary diffusion under steady state conditions. They carried out two analyses: the first was for a single phase material and the second was in a dissimilar or two-phase medium. These authors looked at the elastic properties of the material during crack growth and assumed that no nucleation occurred and that diffusion was the main growth mechanism.

Nguyen et al., (1998), used a small-scale microstructural approach to consider a pre-existing crack under steady-state creep conditions. The authors assume that the damage is developed in a process zone that is much smaller than all relevant specimen dimensions. In this model the authors have defined a ‘process window’ which is situated at the crack tip. Here the grains are represented discretely using what the authors call ‘grain elements’. These are connected by grain boundary elements that describe the fracture mechanisms such as viscous grain boundary sliding, the nucleation of grain boundary cavities, their growth by grain boundary diffusion and by creep of the surrounding material and their final coalescence leading to microcracks. They use a ‘smeared out’ approach as opposed to modelling actual cavity shapes. The process window is surrounded by a continuum discretized by standard creeping elements. The continuum is much larger than the process window so that the near-tip damage does not perturb the far fields. The main aim of this

Figure 20. Cavitation occurs on the boundaries ahead of the crack tip.
Thouless et al. (1983)
paper was to use higher-order crack-tip fields in order to account for the effect of specimen geometry and loading configuration. The model uses an empirical based nucleation law and the growth rate is defined in terms of the average separation between the two adjacent grains. The rate of change of average separation is determined by the volumetric growth rate \( \dot{V} \), and the rate of change of cavity spacing \( \dot{b} \). This model assumes that there is a pre-existing dominant crack, and does not model the damage accumulation process associated with the formation of the crack. This model also has the disadvantage of not being able to model the de-bonding of the grains, that is, the process when they become so ‘damaged’ that they coalesce with the crack tip and the crack then propagates.

The main shortcomings of the models listed here, are:

1. The assumption of fast surface diffusion in the cavities ahead of the crack-tip causing them to remain spherical.
2. No nucleation of cavities during the lifetime of the model, this assumes that the number of cavities is constant, and as one coalesces with the crack-tip a new one is added at the other end.
3. The assumption of steady-state growth of the crack cannot be justified.
4. The models assume that there is a dominant crack already present in the material and model it’s propagation, they do not model the damage accumulation associated with the formation of the crack.
CHAPTER 3. LITERATURE REVIEW

3.7 Computer simulation of cavity and crack growth by solid state diffusion.

3.7.1 Numerical technique.

Recently, a full numerical solution technique has been developed by Cocks and his coworkers (Cocks, 1989), Cocks, Gill and Pan (1999), Pan et al., (1997), Kucherenko and Pan (1998). The full numerical solution can follow the detailed morphological evolution of any cavity shape, it is not limited by the geometry of the cavity as in the simplified models which use an arc or some other shape to approximate the cavity. Using this method it is possible to supply the initial cavity profile which can be of any shape, and then the evolution of the profile can be followed in detail. This method models evolution by a combination of grain boundary diffusion, grain boundary migration and free surface diffusion, and can be readily extended to include other mechanisms which effect the cavity evolution. The method is based on a unified variational principle that allows fully coupled processes to be analysed. The numerical solution provides the velocities of each individual grain and the velocities of grain boundaries and migrating surfaces. When combined with a time integration algorithm, the finite element formulations form a numerical technique that can be used to simulate microstructural evolution in polycrystalline materials. However, due to the complexity of this approach it would be difficult to use the method directly to simulate multiple cavity growth on a grain boundary. Here, hundreds of cavities can be nucleated along a single grain-boundary during the process of creep failure. The number of degrees of freedom of the full numerical model would be unacceptable even for the most powerful workstations currently available.

3.7.2 Cavity growth models.

The model by Cocks, Gill and Pan, (1999) and Pan et al., (1997) uses the full finite element solution to analyse cavity growth. The model takes into account the effects of grain boundary and surface diffusion and produces very detailed evolutions of the cavity profile under varying applied conditions. The model used by van der Giessen and Tvergaard, (1994) analysed the linking up of grain boundary micro-cracks to form a
macroscopic crack. The model accounted for power-law creep and elasticity inside the grains, and assumed that intergranular failure occurred by cavity nucleation and growth to coalescence or by grain boundary sliding. This model does not follow the evolution of individual cavities, but employs a smeared out approach (first introduced by Rice, 1981), in which the individual cavities are replaced by a continuous area of void. The model presented is a 2-D polycrystal consisting of a doubly periodic array of hexagonal grains. The authors state that the simple model estimates of time to microcrack formation tend to be on the high side, this is due to the interaction with other failure mechanisms not being fully accounted for. A more detailed review of this model is given in chapter 6.

Recently the classical Galerkin and Rayleigh-Ritz methods have gained attention for the problems of microstructural evolution. Material interfaces are approximated by simplified profiles with a few degrees of freedom and the virtual power principle or the variational principle is used to obtain the rate equations for the degrees of freedom. This method was used by Sun et al. (1996), to study the sintering kinetics of a row of grains, by Cocks and Gill, (1996), to study grain growth and by Svoboda and Riedel, (1995), to study sintering of powder compacts. It is important to point out that the accuracy of these approximate solutions can only be known when the approximate solutions are compared with full numerical solutions, this is due to the fact that very crude profiles were often assumed for the material surface in the simplified models.

3.7.3 Crack tip fields and crack growth.

Using their numerical technique, Cocks and Pan, (1993) examined the process of void growth ahead of a dominant crack in a material, which deformed by grain boundary diffusion. They limited their attention to a ceramic system where diffusional processes are generally responsible for deformation and void growth. The crack advances by a grain facet length increment when the void adjacent to the crack tip reaches a critical size. There were two limiting cases investigated: the first was where the voids were assumed to have no effect on the stress field. This implied that the void growth within the damage zone was unconstrained. These models overestimate the local stresses and provide upper bounds to the void and crack growth rates. The second case was assumed to occur when the growth of damage is fully constrained, this gave a lower bound to the void and crack
growth rates. In all cases the assumption was made that surface diffusion was sufficiently rapid to ensure that the cavities maintained a spherical shape. Void growth within a body which contains a dominant crack was investigated, and the results for the damage directly ahead of the crack were compared with the two limiting models and Thouless’ (1983), dislocation model. One of the situations analysed by the authors is shown in Figure 21. It consists of a two-dimensional uniform hexagonal array of grains. They assumed the grains remained rigid and the deformation of the material results from the diffusional transport of matter around the grains, which is accommodated by the free sliding of the grain boundaries. They did not consider the influence of void nucleation or coalescence on the material behaviour and did not evaluate the effect of the calculated void growth rate on creep crack growth.

Figure 21. The 2-D uniform poly-grain structure with a central crack and a single void ahead of the crack tip, Cocks and Pan, (1993).

Figure 22 shows the continuum equivalent of the system without any cavities directly ahead of the crack. The numerical procedures used by the authors are based on a variational principle originally proposed by Needleman and Rice, (1980). These are described fully in the paper by Pan and Cocks, (1993), which looked at the effect of grain size on the stress and velocity fields ahead of a crack in a material which deforms by Coble creep. In this paper it is assumed that no cavities occur. The authors used a recently developed computer package that they called NAD-GB (Numerical Analysis of Diffusion along Grain Boundaries), which has powerful pre- and post processors and allowed problems with large numbers of degrees of freedom to be graphically analysed. As part of this paper they used it to analyse a system with 23296 degrees of freedom.
which consisted of three basic types for each grain. These were: the rigid velocity of the grain, the diffusional flux along the free surfaces and boundary that was shared between adjacent grains and the chemical potential at each triple point.

![Diagram](image)

**Figure 22.** The continuum equivalent to the problem of Figure 21, (Cocks and Pan 1993).

The authors concluded that when the voids are confined to being directly ahead of the crack tip Thouless’s, (1983), dislocation model, captures the major physical features and accurately predicts the void growth rates. They state that the presence of additional damage around the damage zone significantly alters the material response, with the volumetric growth rate found to be very sensitive to distribution of damage within the material.
3.8 Conclusions.

For cavity nucleation there have been two different approaches taken in the literature; the first is a thermodynamically based model; the second uses empirical data as its basis. Both of these models have been used extensively despite the fact that the thermodynamically based models predict a very high 'threshold stress' for nucleation and the empirical based models do not have a sound physical basis. There have been suggestions as to how to remedy the problems with the thermodynamically based argument, such as grain boundary sliding and lenticular shaped cavity nuclei. However, it has been shown that these effects are not sufficient to cure the problem and it remains unsolved. The empirical models predict cavity nucleation at any stress and give results comparable to those observed in actual materials. The main drawback is with the use of material constants in the expressions, these can vary widely between materials and can be adjusted in order to fit experimental data. The problem remains as to how to make the two theories agree. The initial thermodynamic expressions are known to be correct and the empirical based model produces results that agree with observations, it is the process in between which has caused the problems, this is partly due to the fact that the nucleation process is not entirely understood. This work will use an empirically based nucleation law in the cavity growth model, as it is less complex than the analytical based models. The results of this model can also be easily compared with recorded data for a variety of materials giving a simple means of checking the results.

For cavity growth there have been a large number of models in the literature, which give good approximations of observed cavity growth. The main differences are the mechanisms governing cavity growth that can be included. The most important of which are listed below.

- The type of growth i.e. constrained or unconstrained.
- The effects of surface diffusion which allow the cavity to evolve into a crack-like shape under the correct conditions.
- The effects of power-law creep which occur at higher temperatures and involve plastic deformation of the grains.
- The sliding of grain boundaries.
• The 'jacking' effect of grain boundaries.
• Interaction of cavities

The ideal situation would be to include all these effects in a single model, but this would be very difficult and the model would be extremely complex. What has been done instead is to include only the effects which play a major role in the cavity evolution, however, different authors have different ideas as to which processes these are. The problem of constrained or unconstrained cavity growth is only applicable when considering an analytical model. This is because a full numerical model can solve the cavity growth problem in one step, although this is very difficult and instead the analytical models assume either the cavity growth is constrained or unconstrained so that problem is transferred to individual grain boundaries and then solved. This is not an issue when solving the system numerically, and as a result all of the main mechanisms can be included.

There is also the problem of the complexity of the model for an individual cavity. The full finite element method by Pan et al., (1997) can be used to model the cavity surface with a large number of elements. These methods produce very accurate simulations of cavity evolution but are CPU intensive for even a single cavity. This also has implications on the modelling of multiple cavities; it would be very difficult to extend the full FE based model of Pan et al., (1997) to model more than one cavity on a grain boundary as the amount of CPU power it would require would make it impractical. The other models assume that the cavities are spherical and remain spherical throughout the evolution, this has been shown to be inaccurate making these models too simplistic. As a result of the literature review there seems a clear requirement to develop a model which has the correct balance between complexity and CPU requirements. There appear to be three main stages to fulfil this requirement, they are:

1. Develop a simplified single cavity model able to model the majority of mechanisms listed above without requiring large amounts of CPU power.
2. Extend the single cavity model to simulate multiple cavities on a grain boundary.
3. Employ the extended model to simulate the evolution of large pre-existing 'crack-like' cavities.
This work will use the truncated arc approach to approximate each cavity. The mechanisms included in the growth model will be grain boundary diffusion, surface diffusion, 'jacking' effects, grain rotation, interconnection and coalescence effects.

The modelling of creep damage accumulation incorporating all the mentioned mechanisms into a crack growth model has been studied extensively. There have been several different approaches presented here, although they are all bound by certain assumptions. These include: nucleated cavities are spherical and surface diffusion is sufficiently rapid to maintain this, the number of voids on a grain boundary is constant, the growth is steady state and that there is already a dominant crack present. There were also different controlling mechanisms that were considered such as plastic flow enhanced diffusion and diffusion of vacancies to the cavity tip and deposition of the atoms on the grain boundary. Some models did not solve the entire problem and, assuming steady state conditions produced a value for only the crack tip velocity. This project will simulate the evolution of large cracks using a newly developed model. This model will provide a more representative simulation than the exiting models by being accurate enough to include mechanisms such as surface diffusion and continuous random cavity nucleation without requiring a large amount of CPU time.

The final section of the review showed a selection of computer based simulations of cavity and crack growth. The purpose was to show how models are combined with computer programs to simulate the evolution of the cavities and cracks. There are several different approaches used for the solution of the models, as well as the type of models used. Some employed a full finite element method to model the individual cavity evolution, whereas others used a 'smeared out' approach to model the entire grain boundary. All these models have been shown to include certain assumptions as well as having limitations on what can be modeled.
4. A simplified model for a grain-boundary cavity.

4.1 Introduction.

Following the requirements identified in the previous chapter to model the evolution of multiple cavities on a grain boundary, this chapter completes the first stage of the work; the construction of a simplified single cavity model that can simulate the effects of surface and grain boundary diffusion.

Following Sun et al., (1996), who modelled the evolution of a row of grains using the dihedral angle as one of the degrees of freedom, a simplified 2 degree of freedom model is proposed here for cavity growth along a grain-boundary by surface and grain-boundary diffusion. The simplified model is justified by comparing it with the full finite element model developed by Pan et al., (1997). This justification was not present in the work of Sun et al., (1996). Two arcs of equal radius truncated by the grain-boundary approximate the cavity surface. As surface diffusion proceeds the arcs evolve by changing their radius and the dihedral angle which they make where the cavity surface meets the grain-boundary. The system has only two degrees of freedom (the cavity radius and the dihedral angle). A variational principle for the coupled diffusion problem is used to obtain the rate equations for the two degrees of freedom. The rate equations are then numerically integrated to follow the cavity growth. It is shown that the approximate solution can be used under most practical service conditions for engineering alloys. One of the major advantages of this model is its relative simplicity, this means that the computer processing time is very short. This also allows the model to be extended to simulate multiple cavities along a single grain boundary (the subject of a subsequent chapter).
4.2 Governing equations.

4.2.1 Thermodynamic and kinetic description.

Consider a uniform array of cylindrical cavities equally spaced on a grain boundary that is subjected to a remote stress $\sigma_\infty$ normal to the grain-boundary, this is shown by Figure 23.

![Figure 23. A row of cavities on a grain boundary between two crystals.](image)

The representative unit of this array is shown in Figure 24. Because of symmetry there is no matter exchange between the unit and its neighbours. The remote stress drives matter to diffuse into the grain-boundary from the cavity surface. As matter is taken away from the cavity surface and deposited onto the grain-boundary, a remote velocity, $V_{gb}$, between the two grains on either side of the grain-boundary is produced.

Considering a grain boundary with periodically distributed cavities of equal size, the representative unit shown in Figure 24 is sufficient to describe the problem. The total free energy per unit depth of the system referred to as $G$ consists of three terms:

$$ G = 2\Gamma_s \gamma_s + \Gamma_{gb} \gamma_{gb} - \sigma_\infty L_0 B $$

(4.2-1)
In which $\Gamma_s$ is the top-half length of the free surface and $\Gamma_{gb}$ is the total length of the grain boundary. $\gamma_s$ and $\gamma_{gb}$ are the specific free energies for the free surface and grain boundary respectively, with $L_0$ and $B$ the dimensions of the representative unit as shown in Figure 24.

Figure 24. A representative element of the system.

The system evolves to reduce $G$. Since $L_0, \gamma_s, \gamma_{gb}$ and $\sigma_\infty$ are constants, $G$ can be reduced by changing $\Gamma_s, \Gamma_{gb}$ and $B$. The two surfaces meet the grain boundary at a dihedral angle $\Psi$, which reaches a value $\Psi_e$ in equilibrium. The equilibrium dihedral angle can be determined from the specific surface and grain boundary energies. For a precise model, $\Psi_e$ the dihedral angle should be:

$$\Psi = \Psi_e = 2\arccos\left(\frac{\gamma_{gb}}{2\gamma_s}\right)$$

(4.2-2)

In the approximate model, however, $\Psi$ is taken as a degree of freedom that is allowed to evolve (Sun et al., 1996). The equilibrium between the surface tensions and the grain-boundary tension, which leads to (4.2-2), is satisfied in a variational sense as discussed in the next section.
The evolution of the cavity involves two kinetic processes: surface diffusion and grain boundary diffusion. Let \( J_s \) be the surface flux (i.e. the volume of atoms passing through a unit area along the surface in a unit time), and \( J_{gb} \) be the grain boundary flux (i.e. the volume of atoms passing through a unit area along the grain boundary in a unit time). As described by Sun et al., (1996), the fluxes can be related to driving forces and mobilities of atoms by:

\[
J_s = M_s F_s \tag{4.2-3}
\]

\[
J_{gb} = M_{gb} F_{gb} \tag{4.2-4}
\]

These expressions define the atomic mobility on the free surface and on the grain boundary respectively, where:

\[
M_s = \text{Mobility for surface diffusion.}
\]

\[
M_{gb} = \text{Mobility for grain boundary diffusion.}
\]

\[
F_s = \text{Driving force of surface diffusion.}
\]

\[
F_{gb} = \text{Driving force of grain boundary diffusion.}
\]

The mobilities can be related to the diffusivities by using the Einstein relations

\[
M_s = \frac{D_s \delta_s \Omega}{kT} \tag{4.2-5}
\]

\[
M_{gb} = \frac{D_{gb} \delta_{gb} \Omega}{kT} \tag{4.2-6}
\]

where:

\[
D_s = \text{Surface Diffusivity.}
\]

\[
D_{gb} = \text{Grain Boundary Diffusivity.}
\]

\[
\delta_s = \text{Effective thickness of surface atoms involved in diffusion.}
\]

\[
\delta_{gb} = \text{Effective thickness of grain boundary atoms involved in diffusion.}
\]

\[
k = \text{Boltzmann’s constant.}
\]

\[
T = \text{Absolute temperature.}
\]

\[
\Omega = \text{Atomic volume.}
\]
4.2.2 Variational principle for surface and grain-boundary diffusion.

The coupled surface and grain boundary diffusion is considered as the mechanism for the cavity growth, i.e. matter is taken away from the cavity surface by a diffusive flux $J_s$ and is deposited onto the grain boundary by a grain boundary diffusive flux $J_{gb}$. For the coupled grain-boundary and surface diffusion problem, we have the following variational principle as given by Sun et al., (1996):

Among all the virtual diffusive fluxes that satisfy matter conservation the true fluxes and their associated grain-boundary separation velocity ($V_{gb}$), minimise the functional $\Pi$:

$$\Pi = \hat{G} + 2 \int \frac{J_s^2}{M_s} d\Gamma_s + \int \frac{J_{gb}^2}{2M_{gb}} d\Gamma_{gb}$$

(4.2-7)

in which $M_s$ and $M_{gb}$ are the mobilities for surface and grain-boundary diffusion respectively. $\hat{G}$ represents the time derivative of $G$ which is given by (4.2-8).

$$\hat{G} = 2\dot{\Gamma}_s \gamma_s + \dot{\Gamma}_{gb} \gamma_{gb} - \sigma_{gb} L \dot{V}_{gb}$$

(4.2-8)

It can be shown that the minimisation of $\Pi$ is equivalent to:

a) The kinetic equations for surface and grain-boundary diffusion

$$J_s = M_s \frac{\partial (\gamma_s \kappa_s)}{\partial s} \quad \text{and} \quad J_{gb} = M_{gb} \frac{\partial \sigma_{gb}}{\partial s}$$

(4.2-9)

In which $\kappa_s$ is the curvature of the cavity surface and $\sigma_{gb}$ is the local grain-boundary stress.

b) The equilibrium between the surface tension $\gamma_s$ and the grain-boundary tension $\gamma_{gb}$ where the cavity surface meets the grain-boundary. This leads to a dihedral angle, $\Psi_s$, at the cavity tip, and we have:
\[ \Psi_s = 2 \cos^{-1} \left( \frac{\gamma_{gb}}{2\gamma_s} \right) \tag{4.2-10} \]

c) The equilibrium between the local grain-boundary stress \( \sigma_{gb} \) (normal to the grain-boundary), the remote stress \( \sigma_c \) and surface tension \( \gamma_s \):

\[ \int \sigma_{gb} ds + \gamma_s \cos \Psi_s - \sigma_c L_0 = 0 \tag{4.2-11} \]

And finally:

d) The continuity of the chemical potential where the cavity surface meets the grain-boundary, which is often expressed as:

\[ \sigma_{gb} = \gamma_s \kappa_s, \quad \text{at the cavity tip.} \tag{4.2-12} \]

When constructing approximate solutions using the above variational principle, conditions (a - d) do not have to be satisfied. The approximate solutions, however, have to satisfy matter conservation including the following relationships between the surface flux \( J_s \) and the surface migration velocity \( V_s \):

\[ V_s + \frac{\partial J_s}{\partial s} = 0 \tag{4.2-13} \]

and between the grain-boundary flux \( J_{gb} \) and the grain-boundary separation velocity \( V_{gb} \):

\[ V_{gb} + \frac{\partial J_{gb}}{\partial X} = 0 \tag{4.2-14} \]
4.3 The 2 dimensional model.

4.3.1 Selection of the degrees of freedom for the model.

The cavity surface can be approximated by two circular arcs of radius $R$ truncated by the grain-boundary. The arcs make an intersection angle $\Psi$ with each other where the cavity surface meets the grain-boundary. The representative unit is completely defined by four parameters, i.e. the horizontal dimension of the unit $L_q$, the vertical dimension of the unit $B$, the radius $R$ and the tip angle $\Psi$. Other geometric parameters can be calculated using these parameters as shown below:

Considering the cavity model shown by Figure 24, the cavity half length ($L_1$)

$$L_1 = R \sin \frac{\Psi}{2}$$  \hspace{1cm} (4.3-1)

The centre of the upper arc is located at $(0, -C)$ with the centre of the lower arc at $(0, C)$ in the X-Y co-ordinate system, as shown in Figure 24 with:

$$C = R \cos \frac{\Psi}{2}$$  \hspace{1cm} (4.3-2)

Let $\theta$ be the angle of the normal to the cavity surface at $(X, Y)$ and the symmetry axis. Then

$$X = R \sin \theta$$  \hspace{1cm} (4.3-3)

$$Y = R \cos \theta - C$$  \hspace{1cm} (4.3-4)

The total length of an arc ($\Gamma_x$) is given by:

$$\Gamma_x = \frac{R \Psi}{2}$$  \hspace{1cm} (4.3-5)

The total length of the grain boundary ($\Gamma_{gb}$)is given by:
Chapter 4 A simplified model for a grain-boundary cavity.

\[ \Gamma_{gb} = L_0 - L_1 = L_0 - R \sin \frac{\Psi}{2} \]  

(4.3-6)

The total area of the material \( A_s \) also needs to be calculated.

Using:

Area of an arc = \( \frac{1}{2} \cdot R_2 \cdot \Gamma_s \)

Figure 25. Calculation of area of cavity.

Using Figure 25, the area of the triangle is given by:

\[ A_{\text{tri}} = \frac{1}{2} R \cos \frac{\Psi}{2} \cdot R \sin \frac{\Psi}{2} \]

\[ A_{\text{tri}} = \frac{R^2}{4} \sin \Psi \]  

(4.3-7)

Area of the arc is given by:

\[ A_{\text{arc}} = \frac{R^2 \cdot \Psi}{4} \]

(4.3-8)

Thus, the total area of the material is the total area of the unit minus (4.3-8) less (4.3-7):

\[ A_s = L_0 B - \frac{R^2 \cdot \Psi}{4} + \frac{R^2}{4} \sin \Psi \]

\[ A_s = L_0 B - \frac{R^2}{4}(\Psi - \sin \Psi) \]  

(4.3-9)
We assume the element length $L_0$ to be constant. Matter conservation requires the total area of solid material in the representative unit to remain constant as the cavity grows. Therefore the system has only two independent degrees of freedom, which are taken as $R$ and $\Psi$ in this model.

### 4.3.2 Rate equations for the two degrees of freedom.

To obtain the rate equations for $R$ and $\Psi$, we first express the diffusive fluxes $J_s$ and $J_{gb}$ in terms of $\dot{R}$ and $\dot{\Psi}$, here “…” represents time derivative. The expressions for $J_s$, $J_{gb}$ and $G$ (which is given by (4.2-1)) are then substituted into (4.2-7) so that the functional $\Pi$ is expressed in terms of $\dot{R}$ and $\dot{\Psi}$. Finally, the rate equations are obtained by minimising $\Pi$ with respect to $\dot{R}$ and $\dot{\Psi}$, i.e. by using

$$\frac{\partial \Pi}{\partial \dot{R}} = 0 \quad \text{and} \quad \frac{\partial \Pi}{\partial \dot{\Psi}} = 0$$

(4.3-10)

This procedure is slightly different from that used by Sun et al., (1996). The difference is between the Rayleigh-Ritz method (used here) and the Galerkin method (used by Sun et al., 1996). As shown in Figure 24, the X and Y co-ordinates of the cavity surface are

$$X = R \sin \theta \quad \text{and} \quad Y = R \cos \theta - C$$

(4.3-11)

where $\theta$ is defined in Figure 24. Figure 26 shows how the migration velocity of the cavity surface is derived.

![Figure 26. Derivation of migration velocity and unit vector.](image-url)
It can be shown that the migration velocity can be expressed as (Appendix A):

\[ V_s = \dot{X}n_X + \dot{Y}n_Y \]  

(4.3-12)

where \( \dot{X} \) and \( \dot{Y} \) are the time derivatives of \( X \) and \( Y \) and \( (n_X, n_Y) \) is the unit vector normal to the cavity surface pointing out of the material which is simply

\[ n_X = -\sin \theta \quad \text{and} \quad n_Y = -\cos \theta \]  

(4.3-13)

Using (4.3-12) and (4.3-13), the surface flux can be obtained by integrating equation (4.2-13). There is a full derivation in Appendix B detailing this operation, with only the final equation shown below:

\[ J_s = \mathcal{R} \mathcal{K} \left( \theta - \cos \frac{\Psi}{2} \sin \theta \right) + \frac{\mathcal{R}^2}{2} \sin \frac{\Psi}{2} \sin \theta \dot{\Psi} \]  

(4.3-14)

The grain boundary flux can be obtained using (4.2-14) as:

\[ J_{gb} = V_{gb} \left( L_0 - X \right) \]  

(4.3-15)

Matter conservation where the grain-boundary meets the cavity surface requires that:

\[ \left( J_{gb} \right)_{X-L_0} = 2 \left( J_{gb} \right)_{\theta=\frac{\Psi}{2}} \]  

(4.3-16)

which leads to:

\[ V_{gb} = \frac{1}{L_0 - R \sin \frac{\Psi}{2}} \left[ \mathcal{R} \mathcal{K} (\Psi - \sin \Psi) + \frac{\mathcal{R}^2}{2} (1 - \cos \Psi) \dot{\Psi} \right] \]  

(4.3-17)

Combining (4.3-15) with (4.3-17), the grain-boundary flux is finally expressed in terms of \( \dot{R} \) and \( \dot{\Psi} \) as

\[ J_{gb} = \frac{L_0 - X}{L_0 - R \sin \frac{\Psi}{2}} \left[ \mathcal{R} \mathcal{K} (\Psi - \sin \Psi) + \frac{\mathcal{R}^2}{2} (1 - \cos \Psi) \dot{\Psi} \right] \]  

(4.3-18)

Now we need to calculate \( \dot{\mathcal{G}} \), the time derivative of the free energy, in order to evaluate the functional \( \Pi \) given by (4.2-7). From (4.2-1) we have:
\[ \dot{G} = 2 \dot{\Gamma}_s \gamma_s + \dot{\Gamma}_{gb} \gamma_{gb} - \sigma_n L_0 V_{gb} \] (4.3-19)

\( V_{gb} \) is given by (4.3-17), \( \dot{\Gamma}_s \) and \( \dot{\Gamma}_{gb} \) can be calculated by differentiating equations (4.3-5) and (4.3-6), (the full derivation is given in Appendix B).

However \( \dot{G} \) would be incomplete if the calculation stops here. As shown by Figure 27, a new surface is created and part of the grain-boundary is lost. This occurs at the junction between the cavity surface and the grain-boundary as matter is inserted onto the grain-boundary. A full derivation of the free energy change due to grain boundary opening is given in Appendix B.

\[ \Delta S_{gb} = \text{Change in grain boundary area.} \]
\[ \Delta S_f = \text{Change in free surface area.} \]

Figure 27. Free energy change due to grain boundary opening.

The main expressions that come from the derivation are shown below. The rate of exchange of free energy at the junction is related to \( V_{gb} \). Kucherenko and Pan, (1998) and Pan et al., (1997) calculated it to be given by:

\[ \dot{G}_{\text{junction}} = \left[ \frac{\gamma_s}{\sin \frac{\Psi}{2}} - \frac{\gamma_{gb}}{2 \tan \frac{\Psi}{2}} \right] V_{gb} \] (4.3-20)

If \( \Psi \) is the dihedral angle given by (4.2-2), (4.3-20) reduces to a more familiar expression:
\[ \dot{G}_{\text{junction}} = \gamma_s \sin \left( \frac{\Psi}{2} \right) V_{gb} \] (4.3-21)

Which is simply the work rate done by the surface tension as the grain-boundary "opens up". \( \dot{G}_{\text{junction}} \) was not included in the work of Sun et al., (1996), although it is important for the problem considered there due to the fact that no external force was considered. For the problem considered in this work, the contribution from the external force (the last term of (4.3-19)) often dominates \( \dot{G} \).

\( \dot{G} \) is calculated fully in Appendix B using (4.3-17), (4.3-19), (4.3-20) and (4.3-1). The expressions of \( \dot{G}, J_s \) and \( J_{gb} \) (given by (4.3-14) and (4.3-18)) are then inserted into the functional \( \Pi \) of (4.2-7), from this we obtain:

\[ \Pi = \frac{1}{2} \left[ \dot{R} \begin{bmatrix} A_{RR} & A_{RP} \\ A_{PR} & A_{PP} \end{bmatrix} \begin{bmatrix} \dot{R} \\ \dot{\Psi} \end{bmatrix} + \begin{bmatrix} B_R \\ B_\Psi \end{bmatrix} \begin{bmatrix} \dot{R} \\ \dot{\Psi} \end{bmatrix} \right] \] (4.3-22)

In which \( A_{RR}, A_{RP} \) and \( A_{PP} \) form the viscosity matrix and \( B_R \) and \( B_\Psi \) are the force vector. The derivations are shown fully in Appendix B. Using (4.3-10) we finally obtain the rate equations for \( \dot{R} \) and \( \dot{\Psi} \):

\[ \begin{bmatrix} A_{RR} & A_{RP} \\ A_{PR} & A_{PP} \end{bmatrix} \begin{bmatrix} \dot{R} \\ \dot{\Psi} \end{bmatrix} + \begin{bmatrix} B_R \\ B_\Psi \end{bmatrix} \begin{bmatrix} \hat{R} \\ \hat{\Psi} \end{bmatrix} = 0 \] (4.3-23)

Which can be integrated numerically giving the time history of \( R \) and \( \Psi \). This concludes the section on obtaining the rate equations for the system and the methods used to solve the system.

### 4.3.3 The 'jacking' effect.

As discussed in the literature review (section 3.5.2), the rigid separation of the grains on either side of the grain boundary leads to a further growth of the cavity. This is referred to
as the jacking effect, which is shown in Figure 29. The jacking effect has not been included in the 2 degrees of freedom, $\dot{R}$ and $\dot{\Psi}$. This is because the rigid motion of grains has to be excluded from the expression of the surface migration velocity $V_s$ for equation (4.2-12), i.e.

$$V_s + \frac{\partial J^g}{\partial s} = 0$$

to be valid. The exclusion of the rigid motion is ensured by using flux conservation, (4.3-16):

$$\left(J_{gb}\right)_{\kappa=b_1} = 2\left(J_{s}\right)_{\sigma=\Psi/2}$$

instead of the volume conservation of the solid material in the representative unit when relating the grain boundary separation velocity $V_{gb}$ to $\dot{R}$ and $\dot{\Psi}$.

In order to calculate the 'jacking' effect, the dihedral angle can be further modified based on the grain boundary separation velocity $V_{gb}$ in addition to the $\Psi$ obtained from solving (4.3-23). As shown in Figure 29 and Figure 30, the extra increment of $\Psi$ caused by the 'jacking' effect can be related to $V_{gb}$ such that:

$$\frac{R}{2} \left(\Delta \Psi\right)_{jacking} \sin \frac{\Psi}{2} = \frac{V_{gb}}{2} \Delta t$$

(4.3-25)

---

1 The volume conservation can be expressed as (see Equation 4.3-9)

$$\frac{dA_s}{dt} = L_0 \frac{\dot{B}}{2} - \frac{R}{2} (\Psi - \sin \Psi) \dot{R} - \frac{R^2}{4} (\dot{\Psi} - \dot{\Psi} \cos \Psi) = 0$$

Noticing that $2 \dot{B} = V_{gb}$, we have:

$$V_{gb} = \frac{1}{L_0} \left[ R \ddot{R} (\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \dot{\Psi} \right]$$

(4.3-24)

This is different from Equation (4.3-17), which was obtained from the flux conservation. As indicated above, Equation (4.3-17) instead of (4.3-24) should be used in the model formulation as (4.3-24) contains the effect of rigid motion of the grains.
hence, we have:

\[
(\Delta \Psi)_{jacking} = \frac{V_{gb} \Delta t}{R \sin \frac{\Psi}{2}} \tag{4.3-26}
\]

The above scheme of including the 'jacking' effect is inappropriate at the extreme of very fast surface diffusion. This is simply because at the extreme of fast surface diffusion, the dihedral angle always maintains its equilibrium value \( \Psi_{\text{e}} \). The extra growth of the cavity caused by the grain boundary separation is better represented by an extra change of \( \dot{R} \).

\[
\Delta A_{\text{extra}} = V_{gb} \cdot \Delta t \cdot R \sin \frac{\Psi}{2}
\]

**Figure 28. Additional change of R due to the 'jacking' effect at the extreme of fast surface diffusion.**

Figure 28 shows how the extra area is calculated. The extra change in radius is calculated once the rates of change of \( R \) and \( \Psi \) have been found. Using (4.3-17), the separation velocity can be calculated. From Figure 28 it can be seen that:

\[
A_{\text{extra}} = V_{gb} \cdot \Delta t \cdot R \sin \frac{\Psi}{2} \tag{4.3-27}
\]

Using (4.3-9) we know that the area of the cavity is:

\[
A = \frac{R^2}{2} \left( \Psi - \sin \Psi \right) \tag{4.3-28}
\]

Assuming that \( \Psi \) is constant, we take the time derivative of (4.3-28), giving:

\[
(\Delta A)_{jacking} = R(\Delta R)_{jacking} \left( \Psi - \sin \Psi \right) \tag{4.3-29}
\]
Equating (4.3-27) with (4.3-29) we have:

\[ V_{gb} \Delta t R \sin \frac{\Psi}{2} = R(\Delta R)_{jacking} (\Psi - \sin \Psi) \]

Therefore:

\[ (\dot{R})_{jacking} = \frac{V_{gb} \sin \frac{\Psi}{2}}{(\Psi - \sin \Psi)} \]  

(4.3-30)

For a situation that is between the two extremes of fast surface and fast grain boundary diffusion, it is difficult to determine which of these two extra modifications to \( \dot{R} \) and \( \Psi \) should be used to include the 'jacking' effect. In this work we always modify \( \dot{\Psi} \) unless we need to push the 2 degree of freedom model to the fast surface diffusion extreme to compare with the 1 degree of freedom model.

![Diagram](Figure 29. Additional change in Dihedral angle due to 'jacking' effect.)
4.3.4 Timestep control within computer routine.

This section looks at the method used to control the size of the timestep in the computer routine, this was in order to maximise the accuracy and prevent the processing time from becoming excessively long. We use the explicit Euler integration scheme for the time integration. It is well known that the direct Euler scheme places a very strict limit on the time step length to obtain a convergent solution. Due to the fact that the rate of cavity growth can vary significantly in the process, it is necessary to use an adaptive timestep for this work. The method used was quite straightforward, the size of the timestep was calculated at each iteration according to the rate of change of each degree of freedom (\( R \) and \( \Psi' \)). These were combined to give a value for the rate of change of the half cavity length (\( \dot{L}_i \)), and it was this that was used to determine the size of the timestep. Using (4.3-1), the method is shown below:

\[
L_i = R \sin \frac{\Psi}{2} \quad \therefore \quad \dot{L}_i = \dot{R} \sin \frac{\Psi}{2} + \frac{R}{2} \cos \frac{\Psi}{2}\]

\[\text{(4.3-31)}\]

Let \( R_0 \) represent a characteristic length of the problem, the initial radius for example, the adaptive time step length \( \Delta t \) is determined such that:

\[
\Delta t \dot{L}_i \leq \alpha R_0 \]

\[\text{(4.3-32)}\]

where \( \alpha \) is an empirical constant.
The value of $\alpha$ was only determined by trial and error. Shown in Figure 31 is a graph, which shows the effect of $\alpha$ on the value of the predicted cavity radius over time. In this example, $R_0$ is chosen to be the initial cavity radius. It can be seen from the chart that an alpha value of 0.1 does not give an accurate result in terms of the time it takes the cavity to evolve. As the value of $\alpha$ is reduced the difference between each set of results is decreased. This occurs until the value of 0.0005 is reached, a further reduction to 0.0001 cannot be distinguished from the previous value.

This shows that, after a certain value has been reached there is no benefit in making $\alpha$ smaller the change in accuracy will be negligible. Therefore 0.0005 was chosen as the value of $\alpha$ that was used in compiling the 'Validity Map' reported in section 4.4.

4.3.5 Non-dimensionalisation of rate equations.

It is convenient to present the results in a non-dimensional form. We therefore choose the initial radius of the cavity $R_0$ as the characteristic length and define $\dot{\varepsilon}_x$ as the characteristic 'strain rate' given by Equation (4.3-33). This has the required units of $1/time$ that allows the actual time to be non-dimensionalised.
\[ \dot{\varepsilon}_s = \frac{M_s y_s}{R_0^4} \]  

(4.3-33)

Using (4.3-33) we can define \( 1/\dot{\varepsilon}_s \) as the reference time \( \tau_g \), and then adopt the following non-dimensionalisations:

\[ \tilde{t} = \frac{t}{\tau_g} \]  

(4.3-34)

\[ \overline{R} = \frac{\tau_g \dot{R}}{R_0} = \frac{\dot{R}}{\dot{\varepsilon}_s R_0} \]  

(4.3-35)

\[ \overline{\Psi} = \Psi \frac{\tau_g}{\dot{\varepsilon}_s} \]  

(4.3-36)

Using the explicit time integration scheme given in section 4.3.5, the evolution of \( R \) and \( \Psi \) can be followed step by step until failure of the grain boundary occurs for the given initial conditions of \( \left( \frac{R_0}{L_0}, \Psi_c \right) \), as well as the kinetic parameters such as the surface and grain boundary mobilities and the specific energy terms. Therefore, the crack profile, the crack propagation and the remote deformation velocity can be determined.
4.4 Validity map of the 2 degree of freedom model.

To investigate the validity of the 2 degree of freedom model, the full finite element numerical technique developed by Pan et al., (1997, 1998), is used to simulate the cavity growth. The numerical technique is based on the same variational principle described in section 4.2.2. The only difference between the numerical solution and the 2 degree of freedom solution is that many degrees of freedom are used in the numerical solution, therefore, complicated cavity profiles can be developed in the numerical simulation.

The full numerical model is then used to judge the validity of the 2 degree of freedom model by comparing the results gained from both solutions. There are several factors which can affect the characteristics of the cavity growth, including:

a) The ratio between the initial size of the cavity and the cavity spacing $R_0/L_0$.

b) The equilibrium dihedral angle $\Psi_e$.

c) The ratio between the applied remote stress $\sigma_{\infty}$ and the 'sintering stress' of the cavity $\gamma_s / R_0$, this can be expressed as a normalised remote stress $\overline{\sigma}_{\infty}$:

$$\overline{\sigma}_{\infty} = \frac{\sigma_{\infty} R_0}{\gamma_s}$$

(4.4-1)

d) The ratio between the surface diffusion mobility $M_s$ and the grain boundary mobility $M_{gb}$.

A large $R_0/L_0$ leads to interaction between the cavities. This is avoided for the purpose of this work and a small value of $R_0/L_0 = 0.1$ is used in this report to simulate isolated cavities. The simplified model is compared with the numerical model for $\Psi_e = 120^\circ$, $150^\circ$ and $180^\circ$, for $\overline{\sigma}_{\infty} = 0 - 50000$ and for $M_{gb}/M_s = 0.0001 - 100$. A total number of 60 cases are used to make the comparison, covering the different combinations of $\Psi_e$, $\overline{\sigma}_{\infty}$ and $M_{gb}/M_s$. 
A characteristic time for the cavity growth can be defined as the time taken by the cavity length ($L_1$ as shown in Figure 24) to reach 60% of the unit dimension $L_0$. The 60% value is chosen because it is found that the interaction between the cavities becomes significant after the cavity grows beyond this stage. If the characteristic time obtained from the simplified model is within ±10% of that obtained from the numerical model, then the simplified model is considered as valid. Based on the comparison, a 'Validity Map' for the simplified model is constructed which is shown in Figure 32.

![Validity Map for dihedral angles of 120°, 150° and 180°.](image)

The map is set out with the normalised remote stress $\bar{\sigma}_n$ on the y-axis, and the ratio of grain boundary mobility $M_{gb}$, to surface mobility $M_s$, on the x-axis. The graph is plotted on a logarithmic scale due to the large range of stresses and mobility ratios that are considered. There are two main areas of interest on the map: the 'Valid Zone' and the 'Invalid Zone'. The 'Valid Zone' is the area under the lines for each dihedral angle, and the 'Invalid Zone' is the area above the lines. We are interested in the range of values underneath the lines, as they indicate what type of conditions this simplified model can simulate accurately.

For each equilibrium dihedral angle, a boundary line is presented on the map, below which the 2 degree of freedom model is valid. It can be seen that the dihedral angle is not a significant factor in determining the validity of the 2 degree of freedom model. The
boundary lines for $\Psi_c = 120^\circ$ and $150^\circ$ are very similar. They both have the same general shape, as well as starting and finishing on approximately the same values for normalised remote stress and ratio of mobility. The boundary line for $\Psi_c = 180^\circ$ is also very similar with the other two if $M_{gb}/M_g$ is less than 0.1. This result should be interpreted carefully as this is a very unrealistic value for a dihedral angle, it could also be possible for a numerical instability to be causing this problem due to the value of $\Psi$. In general, the simplified model becomes invalid for large values of either $M_{gb}/M_g$ or $\bar{\sigma}_\infty$.

To demonstrate if the validity region of the simplified model is relevant to practical conditions, which an engineering component is typically subjected to, we need to put actual material data on the 'Validity Map'. It is difficult to obtain reliable data for material parameters such as grain-boundary and surface diffusion coefficients. Appendix C gives calculated relative diffusion mobilities using data from Ashby, (1990), Chuang et al., (1979) and Riedel, (1987) for a range of materials at $0.5 \times$ melting temperature and $0.8 \times$ melting temperature.

Using $\gamma_s = 1.5 \text{ J/m}^2$ and assuming an applied stress range of 200 – 500 MPa, the normalised stress $\bar{\sigma}$ can be estimated from equation (4.4-1) for a cavity nucleated at a initial size of $R=10 \text{ nm}$ and growing to a size of $R=0.3 \mu \text{m}$. This is shown below:

For applied stress of 200 MPa and a cavity radius of $1\times10^{-9} \text{ m}$:

$$\bar{\sigma}_\infty = \frac{200 \times 10^6 \times 1 \times 10^{-9}}{1.5} = 0.133$$

For applied stress of 500 MPa and a cavity radius of $3\times10^{-7} \text{ m}$:

$$\bar{\sigma}_\infty = \frac{500 \times 10^6 \times 3 \times 10^{-7}}{1.5} = 100$$
This value of normalised stress is shown on the ‘Validity Map’ as the horizontal line. Any location above this line would mean that a stress larger than 500 MPa was being applied, which would be unlikely to occur in most engineering applications.

From the ‘Validity Map’ it can be seen that these values of $M_{gb}/M_s$ and $\bar{\sigma}_e$ are well within the valid zone of the simplified model.

4.4.1 Reduction to the one degree of freedom model at the fast surface diffusion extreme.

At the extreme of fast surface diffusion, the 2 degree of freedom model of equation (4.3-23) can be reduced to a 1 degree of freedom model since $\Psi$ is zero at this extreme. This allows an analytical expression for $\dot{R}$ to be obtained. The analytical expression can be used to check the correctness of the computer implementation of the 2 degree of freedom model by setting $M_s>>M_{gb}$ in the computer program. These results can also be compared with the full finite element solution using many degrees of freedom at this extreme to provide further confirmation of the simplified models. At the extreme of fast surface diffusion, the cavity maintains its equilibrium shape as it grows.

Figure 33. System used in derivation of analytical 1 degree of freedom model.

Figure 33 shows the geometry in this case. It can be shown that at this extreme, (see Appendix D), we have:
in which $l = L_0 - R \sin(\Psi_e / 2)$. When deriving (4.4-2), the effect of grain-boundary separation on cavity growth is included by modifying $\dot{R}$ using the extra growth mechanism. Equation (4.4-2) is only valid at the fast surface diffusion extreme, which is consistent with modifying $\dot{R}$. When comparing (4.4-2) with (3.5-8) it should be noted that $R = a$, $l = b$, $\theta = \Psi$ and $M_{gb} = D_{gb} \delta_{gb} Q_a / kT$. It was found that the two models were in complete agreement under similar conditions. For a full discussion of the ‘jacking’ effect, see section 4.3.4.

Notice that the mobility for surface diffusion, $M_s$, is retained in equation (4.4-2), although the equation is only valid when $M_s \gg M_{gb}$. This is for the purpose of comparing it with the 2 degree of freedom model, since large but finite values of $M_s$ can be used to reduce (4.3-23) numerically to the extreme of fast surface diffusion. In such cases, the energy dissipation by surface diffusion is significant but small.

This model was used to compare the shape of the cavity profile with the full FE-FD model as well as the 2 degree of freedom model. However, due to the nature of the full model and the fact that the cavity profile is made up of finite elements, there is no distinct value of radius ($R$) produced. Therefore, in order to make a meaningful comparison, the half cavity length was calculated at each stage using each of the three models.

Figure 34 shows the cavity profile evolution for an applied stress of 500, $M_s = 1.0$ and $M_{gb} = 0.0003$. It can be seen that in this case the cavity is growing in a self-similar manner and the 1 degree of freedom model agrees well with the other 2 models. Figure 37 shows the evolution of half cavity length for the same conditions. It can be seen that there is close agreement between all three models for the majority of the time, except towards the end of the cavity evolution. Here there is an acceleration in growth rate and the cavity
ceases to be self-similar. It can be seen that the 1 degree of freedom model cannot model this correctly and begins to fall behind. This is further illustrated in Figure 40, where the cavity develops a ‘nose’ almost immediately. The 1 degree of freedom model cannot simulate this and the cavity produced is the wrong shape and also too short. For a more in depth comparison see section 4.5.

The comparisons between the simplified 2 degree of freedom model and the analytical model provided a confirmation for the simplified 2 degree of freedom model.
4.5 Comparison between 2 degree of freedom model and full finite element solution.

This section documents how the 2 degree of freedom model, the 1 degree of freedom model and the full numerical model were compared with each other, using the evolution of the cavity profile and half cavity length. The results are shown in the form of cavity profile evolutions for each model as well as the change in cavity half-length with time for each model.

Although a wide range of applied stresses and mobility ratios were used, only five separate cases are discussed. These are labelled A, B, C, D and E on the ‘Validity Map’ shown by Figure 32. This will show the effect of varying the applied stress while keeping the mobility ratio constant on different dihedral angles. The effect of varying the mobility ratio’s while keeping the applied stress constant is also shown. This has been performed in order to allow direct comparison between the three dihedral angles used (120°, 150° and 180°).

4.5.1 Normalised applied stress=500, \( M_g=1.0, M_{gb}=3\times10^{-4} \).

This case (shown by A in Figure 32), is intended to show that all three models can be valid under certain conditions. Here there is a relatively low applied stress coupled with very fast surface diffusion, due to this, the 2 degree of freedom model uses the modification discussed in section 4.3.3, in order to be comparable with the 1 degree of freedom model. This means that the cavity evolution is controlled by grain boundary diffusion. Therefore the cavity should grow in a self-similar manner for the majority of the time. This is the type of growth which the 1 degree of freedom model can accurately predict and so it should be in close agreement with the 2 degree of freedom model and the full numerical model. Figure 34 shows the cavity evolution with an initial dihedral angle of 120°, the three different models are all shown, and it can be seen that they are all in close agreement for the four times shown. It can be seen that, at time \( \bar{t}=1.23\times10^2 \), the 1 degree of freedom model is beginning to fall behind the other two models, this is due to the fact that the
cavity has ceased growing in a self-similar manner and is starting to develop a ‘nose’. This is something that it cannot model accurately and, as a result, cannot keep pace with the other two models.

...... Full FE-FD model
--2 degree of freedom model
---1 degree of freedom model

Figure 34. Cavity evolution for $\sigma =500$, $M_r = 1.0$, $M_{gb} = 0.0003$, $\Psi = 120^\circ$.

Figure 35 shows the cavity evolution for an initial dihedral angle of $150^\circ$. It can be seen that the three models are in close agreement, with all the cavity profiles being similar in overall area and shape. Again, it is evident that towards the final stages of cavity growth
the 1 degree of freedom model begins to fall behind in terms of cavity growth, this is due to the cavity ceasing to be self-similar.

Figure 35. Cavity evolution for \( \sigma = 500, M_s = 1.0, M_{gb} = 0.0003, \Psi = 150^\circ \).

Figure 36 shows the cavity evolution for an initial dihedral angle of 180°. It can be seen that there is very good agreement at all three time intervals shown, however this is to be expected, as the spherical cavity reduces the 2 degree of freedom model to the form of the 1 degree of freedom model.

Figure 37, Figure 38 and Figure 39 show graphs of the evolution of half cavity lengths for each of the three dihedral angles discussed above. The graphs are intended to give a quantitative view of how the three different models compare in terms of the evolution of the half cavity length. It can be seen that the three graphs are all very similar in
appearance and at the comparison length of 60%, they are all well within 10% of the value from the full numerical model. In fact the 2 degree of freedom model for the 120° dihedral angle is within approximately 6% of the full solution, whereas for the other two dihedral angles it is within approximately 8%. The 1 degree of freedom model is further away at this stage due to the cavity being non-self-similar. However, for all three of the dihedral angles, the maximum difference between the 1 degree of freedom model and the full model is approximately 17%.

Figure 36. Cavity evolution for $\sigma = 500, M_s = 1.0, M_{gb} = 0.0003, \Psi = 180^\circ$. 
Figure 37. Evolution of half cavity length for $\sigma=500$, $M_s=1.0$, $M_{gb}=0.0003$, $\Psi=120^\circ$.

Figure 38. Evolution of half cavity length for $\sigma=500$, $M_s=1.0$, $M_{gb}=0.0003$, $\Psi=150^\circ$. 
The three different dihedral angles have been shown to exhibit very similar behaviour under these conditions. In terms of validity with the 2 degree of freedom model they are all equally valid. This indicates that in this case the initial dihedral angle has very little effect on the accuracy of the 2 degree of freedom model.

4.5.2 Normalised applied stress $\sigma=500$, $M_s=1.0$, $M_{gb}=0.0003$, $\Psi'=180^\circ$.

This case (shown by B in Figure 32), is designed to show the effect of holding the stress constant and increasing the grain boundary mobility in comparison with the previous case. This has the effect of reducing the relative rate of surface diffusion and causing the cavity to grow in a non-self-similar manner from the beginning. This is due to the material which is being drawn away, not being fast enough to be taken from the entire surface, instead it is taken away locally from the tip of the cavity, this causes the cavity to ‘nose’. Therefore this case should demonstrate the 2 degree of freedom ability to model this ‘nosing’ of the cavity, and also the 1 degree of freedom’s inability to do so, hence showing the limitations to the simple analytical model.
Figure 40 shows the cavity evolution for an initial dihedral angle of 120°. It can be seen that the 2 degree of freedom model is very similar to the full numerical model for all the time intervals shown, in both overall shape as well as half cavity length. This highlights the fact that the extra degree of freedom allows the model to accurately predict the growth of the cavity. The 1 degree of freedom model can also be seen in the figure, it is clear to see that it is unable to model this type of cavity growth, and the cavity produced is the incorrect shape, as well as being much shorter in terms of half cavity length.

Figure 41 shows the cavity evolution for the dihedral angle of 150°. This shows a very similar result to the 120° dihedral angle, the 2 degree of freedom model is very similar, even at time \( \bar{t} = 2.63 \) when the cavity has reached 77% of the grain boundary, the difference is approximately only 2.5%. The 1 degree of freedom model is again unable to
model this type of cavity growth accurately, with the shape and length of the cavity being far removed from the full numerical model's predicted profile.

\[
\begin{align*}
\cdots \text{ Full FE-FD model} \\
\text{2 degree of freedom model} \\
\text{- - - 1 degree of freedom model}
\end{align*}
\]

Figure 41. Cavity evolution for \(\sigma = 500, M_s = 1.0, M_{gb} = 0.01, \Psi = 150^\circ\).

Figure 42 shows the cavity evolution for the initial dihedral angle of 180°. The same is true as before, with the 2 degree of freedom model being very accurate compared to the full numerical model in both shape and half cavity length. At time \(\bar{t} = 3.17\) when the cavity has grown to approximately 77%, there is still only a 2.3% difference between the 2 degree of freedom model and the full numerical model. As in previous comparisons the 1
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The degree of freedom model is very different to the other two models; being approximately 66% shorter at time $\bar{t} = 3.17$ than the full numerical model.

---

Figure 42. Cavity evolution for $\sigma = 500$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 180^\circ$.

Figure 43, Figure 44 and Figure 45 show graphs of the evolution of half cavity lengths for each of the three dihedral angles discussed above. They highlight the similarity between the 2 degree of freedom model and the full numerical model, and also show the 1 degree of freedom model to be invalid under these conditions. Once again it can be seen that the dihedral angle has very little effect on the accuracy of the 2 degree of freedom model when compared to the full numerical model.
Figure 43. Evolution of half cavity length for $\sigma=500$, $M_s=1.0$, $M_{gb}=0.01$, $\Psi=120^\circ$.

Figure 44. Evolution of half cavity length for $\sigma=500$, $M_s=1.0$, $M_{gb}=0.01$, $\Psi=150^\circ$.  

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4.5.3 Normalised applied stress=500, \( M_s = 1.0 \), \( M_{gb} = 1.0 \).

This case (shown by C in Figure 32), is designed to show the effect of holding the stress constant at 500, but increasing the grain boundary mobility by a factor of 100 in comparison with the previous case. In this case the grain boundary and surface mobilities are equal, which means that neither the grain boundary diffusion nor surface diffusion control the evolution, instead; they both contribute to the growth of the cavity. In such cases the cavity tends to ‘nose’ very quickly and in an extreme manner. The only change in the cavity is locally, with all the growth occurring at the tip. This is something the 2 degree of freedom model cannot model and it is expected to be invalid. This is also the case for the 1 degree of freedom model (which is not shown, due to its inaccuracy). This case is designed to show the limitations of the approximate models, and show that there are conditions that require the full numerical model to accurately predict the cavity growth rate. This case uses a very high applied stress, and is above the normal maximum operating stress of most engineering materials. The purpose of this case is to push the model to the extreme values to test its behaviour.
Figure 46 shows the cavity evolution for the initial dihedral angle of 120°. It can be clearly seen that the tendency to 'nose' occurs almost immediately, with the tip of the cavity changing rapidly and the base of the cavity virtually unchanged. The 2 degree of freedom model is unable to model this, and, as a result starts to fall behind almost immediately. The shape of the cavity that is predicted by the 2 degree of freedom model is also very different from that of the full numerical model. At time $\bar{t}=2.3\times10^{-3}$ the 2 degree of freedom model is approximately 46% shorter than the profile predicted by the full numerical model.

![Cavity evolution for the initial dihedral angle of 120°](image)

Figure 46. Cavity evolution for $\sigma=500, M_s=1.0, M_{gb}=1.0, \Psi=120^\circ$.

Figure 47 shows the cavity evolution for the initial dihedral angle of 150°. The same is true again for this case, the 2 degree of freedom model falls behind almost immediately and cannot match the growth rate predicted by the full numerical solution. At time $\bar{t}=2.3\times10^{-3}$ the 2 degree of freedom model is approximately 40% shorter than the full numerical model’s prediction.

Figure 48 shows the cavity evolution for the initial dihedral angle of 180°. This is a repeat of the two previous cases, with the 2 degree of freedom model being 70% shorter than the full numerical model at time $\bar{t}=4.75\times10^{-3}$. 

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Figure 47. Cavity evolution for $\sigma = 500$, $M_s = 1.0$, $M_{gb} = 1.0$, $\Psi = 150^\circ$.

Figure 49, Figure 50 and Figure 51 show graphs of the evolution of half cavity lengths for each of the three dihedral angles discussed above. It can be clearly seen that, in this particular case the two approximate methods are not suitable for modelling cavity growth, and the full numerical model is required to accurately predict the evolution of the cavity. This case highlights the limitations that the approximate methods have and provide data which was used in the construction of the ‘Validity Map’, shown in Figure 32.
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Figure 48. Cavity evolution for $\sigma=500$, $M_s=1.0$, $M_{gb}=1.0$, $\Psi=180^\circ$.

Figure 49. Evolution of half cavity length for $\sigma=500$, $M_s=1.0$, $M_{gb}=1.0$, $\Psi'=120^\circ$. 
Figure 50. Evolution of half cavity length for $\sigma = 500$, $M_s = 1.0$, $M_{gb} = 1.0$, $\Psi = 150^\circ$.

Figure 51. Evolution of half cavity length for $\sigma = 500$, $M_s = 1.0$, $M_{gb} = 1.0$, $\Psi = 180^\circ$. 
4.5.4 Normalised applied stress=50000, \( M_s = 1.0, M_{gb} = 0.01 \).

This case (shown by D in Figure 32), is also designed to demonstrate the limitations of the approximate methods. This time, instead of keeping the stress constant, it is increased by 2 orders of magnitude to 50000 in comparison with case 4.5.1, while the grain boundary mobility is held constant at 0.01. This will demonstrate the effects of applied stress on the cavity evolution. In this case, due to the large applied stress the surface diffusion will not be fast enough to allow material to be drawn away from the entire surface. As a result the cavity will tend to ‘nose’ as before, thus causing the 2 degree of freedom model to fall behind, highlighting the limit in terms of applied stress that can be used.

\[ \tau = 0.0 \]

\[ \tau = 8.7 \times 10^{-4} \]

\[ \tau = 1.9 \times 10^{-3} \]

\[ \tau = 2.87 \times 10^{-3} \]

\[ \tau = 2.92 \times 10^{-3} \]

\[ \tau = 2.92 \times 10^{-3} \]

**Figure 52. Cavity evolution for \( \sigma = 50000, M_s = 1.0, M_{gb} = 0.01, \Psi = 120^\circ \).**

Figure 52 shows the cavity evolution for the initial dihedral angle of 120°. As in section 4.5.3 the cavity can be seen to develop a ‘nose’ almost immediately, with the base of the cavity remaining unchanged, while all the growth is occurring locally at the tip. At time \( \tau = 2.92 \times 10^{-3} \) the 2 degree of freedom model is approximately 63% shorter than the full numerical method, as well as being a very different overall shape.
Figure 53 shows the cavity evolution for an initial dihedral angle of 150°. This shows the same outcome as the previous case, with the full numerical model developing a 'nose' almost immediately and then all the growth occurring at the tip. The 2 degree of freedom model is 65% shorter than the full numerical solution at time $t = 3.80 \times 10^{-3}$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{cavity_evolution}
\caption{Cavity evolution for $\sigma = 50000$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 150°$.}
\end{figure}

Figure 54 shows the cavity evolution for the initial dihedral angle of 180°. This is the same as the previous two cases and shows the 'nose' developing and then the growth rate accelerating as time passes, with all the growth occurring at the cavity tip. In this case the 2 degree of freedom model is approximately 68% shorter than the full numerical model at time $t = 4.71 \times 10^{-3}$.
Figure 54. Cavity evolution for $\sigma = 50000$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 180^\circ$.

Figure 55, Figure 56 and Figure 57 show graphs of the evolution of half cavity lengths for each of the three dihedral angles discussed above. These graphs show clearly show the limitations of the approximate methods modelling this type of cavity growth. They are very similar to the graphs in section 4.5.3, which also showed the limitations to the approximate methods. Therefore it can be concluded that holding the grain boundary mobility constant and increasing the applied stress has the same effect as holding the stress constant and increasing the grain boundary mobility. The outcome of both, yields cavities which tend to ‘nose’ almost immediately with all the growth occurring at the cavity tip.
Figure 55. Evolution of half cavity length for \( \sigma = 50000, M_s = 1.0, M_{gb} = 1.0, \Psi = 120^\circ \).

Figure 56. Evolution of half cavity length for \( \sigma = 50000, M_s = 1.0, M_{gb} = 1.0, \Psi = 150^\circ \).
4.5.5 Normalised applied stress=10, $M_g=1.0$, $M_{gb}=0.01$.

This is the final case selected here (shown by E in Figure 32), and it is designed to show all three models in close agreement. This continues the series of tests that hold the grain boundary mobility constant and vary the applied stress. In this case the stress has been reduced from 500 to 10 in comparison with case 4.5.1. This should have the effect of allowing the material being drawn away from the cavity surface to be done so instantaneously, thus keeping the cavity self-similar in shape and allowing the 1 degree of freedom model to accurately predict the cavity growth. This effect should be similar to that of holding the stress constant and reducing the grain boundary mobility as in section 4.5.1. This case also requires the modified 2 degree of freedom method to be used as discussed in section 4.3.3, due to the fast surface diffusion and the fact that the radius is changing rapidly instead of the dihedral angle.

Figure 58 shows the cavity evolution for the initial dihedral angle of 120°. It can be seen that all three of the models are in close agreement for the time intervals shown. The figure shows that the cavity is self-similar in nature for this time, and the 1 degree of freedom
model is in close agreement with the other two. At time $\bar{t} = 1.70 \times 10^2$ the half cavity length is within 5.5% of the full numerical model. The two degree of freedom model is even more accurate, being within 0.7% at the same time interval.

\[ \cdots \text{Full FE-FD model} \]
\[ \cdots \text{2 degree of freedom model} \]
\[ \cdots -1 \text{ degree of freedom model} \]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{cavity_evolution}
\caption{Cavity evolution for $\sigma = 10$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi' = 120^\circ$.}
\end{figure}

Figure 59 shows the cavity evolution for the initial dihedral angle of $150^\circ$. There is close agreement between all three models again, at time $\bar{t} = 2.20 \times 10^2$ the 1 degree of freedom model is within 3% of the full numerical solution, and the 2 degree of freedom model is within 0.75%. These are very similar to the results for the dihedral angle of $120^\circ$, indicating that the dihedral angle has very little effect on the evolution of the cavity in this case as well.
Figure 59. Cavity evolution for $\sigma=10$, $M_s=1.0$, $M_{gb}=0.01$, $\Psi=150^\circ$.

Figure 60 shows the cavity evolution for the initial dihedral angle of $180^\circ$. As for the previous two dihedral angles the three models are in close agreement for the time intervals shown. The cavity is still growing in a self-similar manner and the 1 degree of freedom model is in close agreement with the other two models. At time $\tilde{t}=2.40 \times 10^2$ the 1 degree of freedom model is within 2.5% of the full numerical solution and the 2 degree of freedom model is within 0.9%. Again these results are very similar as those for the previous two dihedral angles.
Figure 60. Cavity evolution for $\sigma = 10$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 180^\circ$.

Figure 61, Figure 62 and Figure 63 show graphs of the evolution of half cavity lengths for each of the three dihedral angles discussed above. The graphs show that while the cavity is growing in a self-similar manner all three models are in close agreement with each other. However, when the cavity starts to develop a slight ‘nose’ and ceases to be self-similar, the 1 degree of freedom model begins to fall behind. Again it can be seen that the dihedral angle has very little effect on the accuracy of the approximate models when compared to the full numerical model. These are very similar results to those in section 4.5.1, which indicates that the effect of holding the grain boundary mobility constant and
reducing the applied stress is the same as holding the stress constant and reducing the grain boundary mobility.

Figure 61. Evolution of half cavity length for $\sigma = 10$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 120^\circ$.

Figure 62. Evolution of half cavity length for $\sigma = 10$, $M_s = 1.0$, $M_{gb} = 0.01$, $\Psi = 150^\circ$. 
Figure 63. Evolution of half cavity length for $\sigma=10, M_s=1.0, M_{gb}=0.01, \Psi=180^\circ$.

Figure 64 shows results from the 2 degree of freedom model which highlight the effects of varying the applied stress whilst keeping the dihedral angle, surface mobility and grain boundary mobility constant. It can be seen that the half cavity length propagation curve involves steady state and transient stages, which are clearly continuous. The graph also shows that, as the applied stress is increased the steady state process becomes shorter.

Figure 64. Effect of varying applied stress on cavity growth rate with $R_0=1, L_0=10, \Psi=150^\circ, M_s/M_{gb}=1$. 
4.6 Conclusions.

In this chapter, a simplified model of grain boundary cavities has been constructed. By using the variational principle a set of ordinary differential equations are derived, which govern the evolution of the cavities. This 2 degree of freedom solution is compared with a full Finite Element-Finite Difference (FE-FD) numerical solution by Pan et al., (1997) and Kucherenko and Pan, (1998). It is found that the proposed simplified model accurately describes the evolution process, in terms of overall cavity profile and cavity propagation rate under practical stresses and diffusivities. This is achieved with only two degrees of freedom compared to the many degrees of freedom employed in the FE-FD solution.

Care must be taken when using the well-established quasi-equilibrium model to calculate cavity growth rate because it is only valid at the very extreme of fast surface diffusion. For more practical circumstances, the simplified model presented in this chapter offers a simple and effective alternative.

The major advantage of the 2 degree of freedom model over the full FE-FD numerical solution is the computer processing time required to complete a simulation. The 2 degree of freedom model takes in the order of one to two minutes to complete, whereas the full numerical solution can take several days to complete a simulation. It must be noted however, that this is for one cavity only. It is quite possible to have as many as 300 cavities present on a grain boundary. The simplified model could be used to model this number of cavities without requiring large amounts of processing time. However, the immense processing time required by the full FE-FD solution would make its use impractical.
5. A simplified finite element scheme for the modelling of multiple cavities on a single grain boundary.

5.1 Introduction.

The problem to be considered is the modelling of a single grain boundary with multiple cavities present on it. The effects of coalescence and nucleation are included in the model and are discussed in detail in Sections 5.3 and 5.4. Each cavity is modelled in such a way as to make it a self-contained cavity 'element'. This 'element' is assembled together with many other 'elements' to form a large number of cavities on a single grain boundary. The cavities are then free to grow and interact with each other depending on the parameters applied to the system. During the evolution of the system the damage fraction can be calculated and a time to fracture found.

Figure 65 shows the typical problem that this method can simulate: multiple cavities on a single grain boundary. There can be multiple cavities present before the load was applied or they can be nucleated as the system evolves.

![Figure 65. Multiple cavities on a single grain boundary.](image)

The new simplified finite element model is a further extension of the 2 degree of freedom model in the previous chapter, Westwood et al., (2000). It has been extended so that it
may simulate the interactions between the cavities. The cavities are allowed to 'shift' along the grain boundary and the grains can rotate as well as separate with respect to each other during the evolution. There was also the need for multiple elements to be assembled together to form a global stiffness matrix which can be solved numerically in a classical finite element approach. This approach has the advantage of using a relatively simple model for the cavity evolution, which can be used many times without requiring a large amount of processing power. The cavity 'element' has an increased number of degrees of freedom (6 compared with the 2 degree of freedom model in the previous chapter). The geometry of the new system is shown in Figure 66 as well as a brief description of the degrees of freedom and the extra mechanisms to be modelled. The system that is defined is a complete element and contains one cavity and a length of grain boundary on each side.

![Figure 66. Construction of a cavity element.](image)

It can be seen from Figure 66 that the cavity is modelled using a truncated arc as before, with the radius $R$, and the dihedral angle $\Psi$ being used to control the shape of the profile. The position of the centre of the cavity is referred to as $x_c$, which is allowed to move with time. This was used to keep track of the position of the cavity on the grain boundary. The position of the translational and rotational velocities of the grain is defined at $x = x_g$, where $x_g$ is the global co-ordinate of the translational and rotational velocities. $V$ and $\omega$ are global degrees of freedom; and are shared by all the elements. The lengths of each side of the element are defined using the superscripts (') for the left side and (") for the right side.
The two grain boundary fluxes $J_{g_b}^1$ and $J_{g_b}^2$ are shared with adjacent elements when assembled to form the global stiffness matrix for a large number of cavities on a grain boundary. There is also a free surface flux, which is shown as $J_s^0$ and is positive in a clockwise direction across the centre of the cavity surface.

5.2 Finite element formulation of a cavity element.

5.2.1 The variational principle.

The same variational principle discussed in section 4.2.2 is used here for the multiple cavity problem. The total free energy of the system is referred to as $G$ and is given by:

$$G = 2\Gamma_g \gamma_s + \Gamma_{g_b} \gamma_{g_b} - \sigma_a \left(x^+ + x^-\right) B - M\theta$$  \hspace{1cm} (5.2-1)

In which $\Gamma_g$ and $\Gamma_{g_b}$ are the total lengths of the free surface and grain boundary respectively, $\gamma_s$ and $\gamma_{g_b}$ are the specific free energies for the free surface and grain boundary respectively, with $(x^+ + x^-)$ giving the total length of the element and $B$ giving the height of the element unit as shown in Figure 66. $M$ is the applied torque with $\theta$ giving the relative rotation between the two grains. The element is derived in two halves, which means there is a separate expression for $G$ for the right and left sides. The system evolves to reduce $G$. The two surfaces meet the grain boundary at a dihedral angle $\Psi$, which reaches a value $\Psi_e$ in equilibrium. The equilibrium dihedral angle can be determined by surface energy and grain boundary energy. For a precise model, $\Psi$, the dihedral angle should be:

$$\Psi = \Psi_e = 2\arccos\left(\frac{\gamma_{g_b}}{2\gamma_s}\right)$$  \hspace{1cm} (5.2-2)

In the approximate model, however, $\Psi$ is taken as a degree of freedom that is allowed to evolve (Sun et al., 1996). The equilibrium between the surface tensions and the grain-boundary tension, which leads to (5.2-2), is satisfied in a variational sense as discussed in
the next section. The evolution of the cavity involves two kinetic processes: surface diffusion and grain boundary diffusion. Let $J_s$ be the surface flux (i.e. the volume of atoms passing across a unit area on the surface in a unit time), and $J_{gb}$ be the grain boundary flux (i.e. the volume of atoms passing across a unit area on the grain boundary in a unit time).

The coupled surface and grain boundary diffusion is considered as the mechanism for the cavity growth, i.e. matter is taken away from the cavity surface by a diffusive flux $J_s$ and is deposited onto the grain boundary by a grain boundary diffusive flux $J_{gb}$. For the coupled grain-boundary and surface diffusion problem, we use the variational principle (Sun et al., 1996)

$$\Pi = \dot{G} + 2 \int \frac{J_s^2}{2M_s} d\Gamma_s + \int \frac{J_{gb}^2}{2M_{gb}} d\Gamma_{gb}$$  \hspace{1cm} (5.2-3)

In which $M_s$ and $M_{gb}$ are the mobility's for surface and grain-boundary diffusion respectively. The expressions shown in Section 4.2.1 relating fluxes to driving forces are used, leading to the following expressions showing how the mobilities are related to the diffusivities:

$$M_s = \frac{D_s \delta_s \Omega}{kT} \hspace{1cm} (5.2-4)$$

$$M_{gb} = \frac{D_{gb} \delta_{gb} \Omega}{kT} \hspace{1cm} (5.2-5)$$

Expressions (5.2-4) and (5.2-5) define the atomic mobility on the free surface and on the grain boundary respectively. $\dot{G}$ represents the time derivative of $G$ which is given by (5.2-3). The above function is applied to each half of the element, and is combined before being solved. When constructing approximate solutions using the above variational principle the approximate solutions have to satisfy matter conservation including the following relationships between the surface flux $J_s$ and the surface migration velocity $V_s$:

$$V_s + \frac{\partial J_s}{\partial \delta_s} = 0 \hspace{1cm} (5.2-6)$$
between the grain-boundary flux $J_{gb}$ and the grain-boundary separation velocity $V_{gb}$

$$V_{gb} + \frac{\partial J_{gb}}{\partial x} = 0 \quad (5.2-7)$$

A brief derivation of the flux terms is given in Sections 5.2.3 as well as the full velocity term incorporating the effects of grain rotation.

### 5.2.2 Selection of the degrees of freedom for the simplified finite element model.

Consider a large number of cavities on a grain-boundary that is subjected to a remote stress $\sigma_n$ normal to the grain-boundary. An example of this is shown in Figure 65. This system is made up from a large number of cavity ‘elements’ that are assembled together to form the global system. One such ‘element’ is shown in Figure 66. As this model is based on the classical finite element approach, each ‘element’ has to share the grain boundary fluxes at each end of the cavity element with the adjacent element. This permits matter to flow between elements when they are assembled and exposed to an applied load. The remote stress drives matter to diffuse into the grain-boundary from the cavity surface. As matter is taken away from the cavity surface and deposited onto the grain-boundary, a remote separation velocity, $V$ and a relative rotational velocity $\omega$, is produced between the two grains on either side of the grain-boundary. The separational and rotational velocities are global degrees of freedom i.e. they are the same for all the cavity elements present in the system. The model can respond to any moment, $M$, that might be applied to the grains. This has been included to model the effects of grain rotation on cavity evolution, and is linked with the ‘shifting’ of the cavities along the grain boundary, that is, an applied moment can cause the cavities to move to the area of grain boundary that is ‘opening up’.

The flux flowing along the grain boundary either side of the cavity is defined as $J_{gb}^1$ for the left-hand side and $J_{gb}^2$ for the right-hand side and varies with position on the grain boundary. These are local degrees of freedom for the element. The degrees of freedom used to model the cavity profile are the same as in the 2 degree of freedom model from
chapter 4. These are the rate of change of cavity radius, \( \dot{R} \), and rate of change of dihedral angle, \( \dot{\Psi} \).

In the simplified finite element model the cavities are allowed to ‘shift’ or translate along the grain boundary. This allows the cavities to be mobile and respond to the applied conditions. The position of the centre of the cavity is defined as \( x_c \), and the first differential is defined as \( \dot{x}_c \), and is the degree of freedom. This gives the rate of change of position of the centre of the cavity and makes it possible to follow the positions of the cavities on the grain boundary. The variable \( \dot{x}_c \) was not required in the 2 degree of freedom model. The reason for the inclusion of \( \dot{x}_c \) is to allow the model to simulate asymmetric systems.

The surface flux \( J^b_s \) is also a degree of freedom, although it is re-written in terms of the remaining degrees of freedom using the second mass conservation term and is shown in Section 5.2.3.

There are 8 degrees of freedom in total, however the use of mass conservation at the left and right hand side cavity tips has reduced this to six. This has the effect of reducing the size of the elemental matrix and so reducing the time required solving the system. These degrees of freedom can be assembled into a global system of simultaneous equations, which can be solved numerically. The degrees of freedom are: 1) separation velocity \( V \), 2) rotational velocity \( \omega \), 3) left grain boundary flux \( J^1_{gb} \), 4) right grain boundary flux \( J^2_{gb} \), 5) rate of change of cavity radius \( \dot{R} \) and, 6) rate of change of position of the centre of the cavity \( \dot{x}_c \).

5.2.3 Formulation of a cavity ‘element’.

The cavity ‘element’ is formed using the variational principal outlined in the previous sections. The element uses it’s own local co-ordinate system that is then mapped onto the global system. The basic system is shown in Figure 67.
Figure 67. Co-ordinate system of cavity 'element'.

Using Figure 67 the local co-ordinate system is defined in terms of the global values. The local co-ordinate expressions are given by \( \zeta_1 \) and \( \zeta_2 \), whereas the global system is defined using the \( x \) and \( z \) terms. Using these definitions it can be seen that, globally:

\[
x = z + x_g\tag{5.2-8}
\]

And the local co-ordinates can be written as:

\[
\zeta_1 = x - (x_c - x^-),\tag{5.2-9}
\]

\[
\zeta_2 = (x_c + x^+) - x,\tag{5.2-10}
\]

Inserting (5.2-8) into (5.2-9) and (5.2-10) we arrive at:

\[
z_1 = \begin{cases} 
\zeta_1 - x_g + (x_c - x^-), & \text{on the left grain boundary} \\
\zeta_2 - x_g - (x_c + x^-), & \text{on the right grain boundary}
\end{cases} \tag{5.2-11}
\]

This defines the position on the grain boundary in terms of the local co-ordinates as well as the global values. The separation velocity is a function of \( V \), \( \omega \) and \( z \), and is given by:

\[
V_{yb} = V + \omega z \tag{5.2-13}
\]
Equations (5.2-11) and (5.2-12) are inserted into (5.2-13) to give separate expressions for the separation velocity for the left and right side of the cavity and using the expression:

$$\frac{\partial J_{gh}}{\partial \zeta} = -V_{gh}$$ (5.2-14)

Integrating (5.2-14) we obtain expressions for the left and right grain boundary flux respectively, which are shown by (5.2-15) and (5.2-16).

$$J_{gh}^1 = -V\zeta_1 - \frac{\omega \zeta_1^2}{2} + \omega x_\zeta \zeta_1 - \omega x_c \zeta_1 + \omega x_c \zeta_1 + J_0^1$$ (5.2-15)

$$J_{gh}^2 = -V\zeta_2 - \omega x_\zeta \zeta_2 + \omega x_c \zeta_2 - \omega x_c \zeta_2 + \omega x_c \zeta_2 + \frac{\omega \zeta_2^2}{2} + J_0^2$$ (5.2-16)

The degrees of freedom have been identified and need to be numbered to enable the local viscosity matrix for each element to follow the same rule. The numbering of the elemental degrees of freedom is shown in Figure 68. This numbering scheme is maintained throughout the system.

![Figure 68. Numbering scheme for elemental degrees of freedom.](image)

The rate equations for the selected degrees of freedom are derived from the expressions for the diffusive fluxes. These are based on the 2 degree of freedom model given in chapter 4, but have additional terms for the new mechanisms being considered. However, before the rate equations can be derived mass conservation has to be satisfied at both cavity tips. This reduces the number of degrees of freedom to six. The right-hand cavity tip is used to
obtain an expression for the surface flux, \( J^0_s \), in terms of the remaining degrees of freedom. The left-hand tip is used to obtain an expression for the rate of change of dihedral angle, \( \Psi \), in terms of the remaining degrees of freedom. The expression for surface flux, \( J_s \), given by Equation (4.3-14) has been extended to simulate the 'shifting of the cavities. Equation (5.2-17) shows the additional \( \dot{x}_c \) term, which permits the rate of change of positions of the cavity centre to be included in the surface flux expression.

\[
J_s = R \hat{R} \left( \theta - \sin \theta \cos \frac{\Psi}{2} \right) - R \dot{x}_c \left( \cos \theta - \cos \frac{\Psi}{2} \right) + \frac{\Psi R^2}{2} \sin \theta \sin \frac{\Psi}{2} + J^0_s \quad (5.2-17)
\]

Using the boundary conditions of:

\[
\theta = \frac{\Psi}{2} \at \text{right tip} \quad \text{and} \quad \theta = -\frac{\Psi}{2} \at \text{left tip}
\]

We arrive at two expressions for the surface flux at the left and right cavity tips. The surface flux must be equal to the grain boundary flux at the cavity tip for mass conservation to be satisfied, hence we equate them with the expressions for grain boundary flux at each of the cavity tips as given by (5.2-15) and (5.2-16). The value of the local coordinate, \( \zeta \), is known at this point, as the total length of the elemental grain boundary, and is written in terms of the global value. Figure 69 shows how the surface and grain boundary fluxes are equated to satisfy mass conservation.

![Figure 69. Example of mass conservation for right-hand side of cavity element.](image)

The surface and grain boundary fluxes are equated using (5.2-18) below:

\[
2J_{s_{\eta'}} = -J_{gb_{\eta'}} \quad (5.2-18)
\]

For the left-hand cavity tip we obtain an expression for the dihedral angle, given by:
\[ \Psi = \frac{2}{A_g R^2} \left[ \dot{\mathbf{A}}_g \mathbf{R} + 2J_0^2 - J_0 + \omega L_1 \right] \]  

(5.2-19)

Where: \( A_g = \sin \Psi - \Psi \), \( A_g = 1 - \cos \Psi \) and \( A_{11} = (L_1/2 - x_g + x_e - x_1) \). A full derivation is given in Appendix E. Incorporating the Equation (5.2-19) as well as using the right hand cavity tip mass conservation, we obtain an expression for the surface flux, given by:

\[ J_s^0 = \frac{1}{4} \left[ VB_9 + \omega A_{31} + J_x - J_x - \dot{\mathbf{R}}_B \right] \]  

(5.2-20)

Where: \( A_{31} = (x_e L_2 x - x_e L_2 - L_2^2/2 - L_1 A_{11}) \), \( B_1 = R(A_{10} + A_9) \) and \( B_9 = L_2 - L_1 \).

Inserting (5.2-20) into (5.2-19) we arrive at the final expression for \( \Psi \):

\[ \Psi = \dot{\mathbf{R}}_{15} B_{18} + VB_{16} B_{18} + \omega B_{17} B_{18} + J_x^0 \frac{B_{18}}{2} + J_x^0 \frac{B_{18}}{2} \]  

(5.2-21)

Where: \( B_{15} = (RA_6 - B_1/2) \), \( B_{16} = B_9/2 + L_1 \), \( B_{17} = A_{31}/2 + L_1 A_{11} \) and \( B_{18} = 2/A_g R^2 \).

The viscosity matrix is derived in stages using the expressions for surface and grain boundary flux as well as the replaced degree of freedom expressions. The contribution from surface flux is calculated by inserting (5.2-17) into the integral shown in (5.2-22), this is carried out for the left and right side of the cavity element, and results in two expressions for the surface flux on the cavity.

\[ 2 \int \frac{J_s^2}{2M_s} d\Gamma_s \]  

(5.2-22)

The same is carried out for the grain boundary terms using equations (5.2-15) and (5.2-16) and the corresponding grain boundary integral given by (5.2-23).

\[ \int \frac{J_{gb}^2}{2M_{gb}} d\Gamma_{gb} \]  

(5.2-23)

The two sets of equations are too long to be included in this chapter, however a full derivation of the viscosity and force matrices is given in Appendix E. The remaining term
to be calculated is the rate of change of free energy of the system, $\dot{G}$, given by (4.3-19). $\dot{G}$ is calculated fully in Appendix E using (5.2-1). The expressions of $\dot{G}$, $J_{gb}$ and $J_s$ are then inserted into the functional $\Pi$ of (5.2-3), from this we obtain:

$$\Pi_e = \frac{1}{2} \left[ X_e^T \right] \left[ A^e \right] \left[ X_e \right] + \left[ B^e \right] \left[ X_e \right]$$  \hspace{1cm} (5.2-24)

where $\Pi_e$ is the contribution from element $e$ to the total $\Pi$. $[A^e]$ is the elemental viscosity matrix, $[B^e]$ is the elemental force matrix and $[X^e]$ contains the elemental degrees of freedom. After applying the appropriate minimizations of the functional we obtain the local viscosity and force matrices:

$$[A_e] = \begin{bmatrix}
A_{vv} & A_{vo} & A_{vi} & A_{ji} & A_{vi} & A_{vo} & A_{ve} \\
A_{ov} & A_{oo} & A_{oi} & A_{oj} & A_{vi} & A_{vo} & A_{oe} \\
A_{iv} & A_{io} & A_{ii} & A_{ij} & A_{vi} & A_{vo} & A_{iv} \\
A_{jv} & A_{jo} & A_{ji} & A_{jj} & A_{ji} & A_{jo} & A_{jv} \\
A_{rv} & A_{ro} & A_{ri} & A_{rt} & A_{rr} & A_{ro} & A_{rv} \\
A_{sv} & A_{so} & A_{si} & A_{st} & A_{sr} & A_{so} & A_{sv}
\end{bmatrix}$$  \hspace{1cm} (5.2-25)

$$[B_e] = \begin{bmatrix}
B_v & B_o & B_{jv} & B_{jv} & B_r & B_{sr} & B_{sv}
\end{bmatrix}^T$$  \hspace{1cm} (5.2-26)

Where (5.2-25) is a positive definite matrix with the diagonal terms dominating and together with (5.2-26), can be assembled into the global viscosity and force matrices using:

$$\Pi = \sum_{e=1}^{n} \frac{1}{2} \left[ X_e^T \right] \left[ A^e \right] \left[ X_e \right] + \sum_{e=1}^{n} \left[ B^e \right] \left[ X_e \right]$$  \hspace{1cm} (5.2-27)

where $e$ denotes the number of the element and $n$ gives the total number of elements. A full derivation of the above method as well as listings of the matrix coefficients is given in Appendix E.

### 5.2.4 Assembly of elements into global system

The cavity elements can be assembled together in the classical finite element approach. The first step is to globally number the degrees of freedom. The numbering scheme is
arbitrary but must be simple as it is automatically generated and updated in the computer model as new elements are added or taken away. Figure 70 shows the numbering system adopted for this model.

\[ \begin{align*}
J_0^1 = 3 & \quad J_0^2 = 6 & \quad J_0^1 = 9 & \quad J_0^2 = 12 & \quad J_0^1 = 15 & \quad J_0^2 = 18 \\
\hat{R} = 4 & \quad \hat{R} = 7 & \quad \hat{R} = 10 & \quad \hat{R} = 13 & \quad \hat{R} = 16 \\
\hat{x}_c = 5 & \quad \hat{x}_c = 8 & \quad \hat{x}_c = 11 & \quad \hat{x}_c = 14 & \quad \hat{x}_c = 17
\end{align*} \]

**Figure 70. Global numbering system for degrees of freedom.**

The global numbering scheme can be seen to be different to the elemental numbering scheme, it is therefore necessary to use a ‘Link’ matrix, which maps the elemental degrees of freedom into the correct position in the global matrix of equations. The following definition of the ‘Link’ matrix is used:

\[ \text{LINK} [i, j] = \text{Global number of degree of freedom of the } i^{\text{th}} \text{ local degree of freedom of element } j. \]

As an example of the link matrix, using the system defined in Figure 70 and the elemental numbering system defined in Figure 68, we have the following values of the ‘Link’ matrix:

\[ \begin{align*}
\text{LINK} [1, 3] & = 1 \quad \text{(Velocity is global and always } 1^{\text{st}} \text{ degree of freedom)} \\
\text{LINK} [3, 3] & = 9 \quad \text{(Since } J_1 \text{ is shared and the } 3^{\text{rd}} \text{ degree of freedom of element } 3)
\end{align*} \]

Once this had been carried out the model was checked for mass conservation to ensure there was no loss of flux under certain conditions. This was part of a large number of tests carried out to ensure the model was behaving as it should. The total number of degrees of freedom in the assembled model was calculated as:

\[ \text{Total degrees of freedom} = 6 \times \text{number of elements} - 3 \times (\text{number of elements} - 1) \]
5.2.5 Solution of the global system.

The structure of the assembled global viscosity matrix for the simplified finite element model is given by Equation (5.2-28). It can be seen that the system is sparsely populated with two rows extending along the top of the matrix and two columns extending down the left-hand side. There is then a band of four elements running diagonally through the centre of the matrix.

\[
\begin{bmatrix}
  a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & a_{1,6} & a_{1,7} & a_{1,8} & a_{1,9} & a_{1,10} & a_{1,11} & a_{1,12} \\
  a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} & a_{2,5} & a_{2,6} & a_{2,7} & a_{2,8} & a_{2,9} & a_{2,10} & a_{2,11} & a_{2,12} \\
  a_{3,1} & a_{3,2} & a_{3,3} & a_{3,4} & a_{3,5} & a_{3,6} & a_{3,7} & a_{3,8} & a_{3,9} & a_{3,10} & a_{3,11} & a_{3,12} \\
  a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} & a_{4,5} & a_{4,6} & a_{4,7} & a_{4,8} & a_{4,9} & a_{4,10} & a_{4,11} & a_{4,12} \\
  a_{5,1} & a_{5,2} & a_{5,3} & a_{5,4} & a_{5,5} & a_{5,6} & a_{5,7} & a_{5,8} & a_{5,9} & a_{5,10} & a_{5,11} & a_{5,12} \\
  a_{6,1} & a_{6,2} & a_{6,3} & a_{6,4} & a_{6,5} & a_{6,6} & a_{6,7} & a_{6,8} & a_{6,9} & a_{6,10} & a_{6,11} & a_{6,12} \\
  a_{7,1} & a_{7,2} & a_{7,3} & a_{7,4} & a_{7,5} & a_{7,6} & a_{7,7} & a_{7,8} & a_{7,9} & a_{7,10} & a_{7,11} & a_{7,12} \\
  a_{8,1} & a_{8,2} & a_{8,3} & a_{8,4} & a_{8,5} & a_{8,6} & a_{8,7} & a_{8,8} & a_{8,9} & a_{8,10} & a_{8,11} & a_{8,12} \\
  a_{9,1} & a_{9,2} & a_{9,3} & a_{9,4} & a_{9,5} & a_{9,6} & a_{9,7} & a_{9,8} & a_{9,9} & a_{9,10} & a_{9,11} & a_{9,12} \\
  a_{10,1} & a_{10,2} & a_{10,3} & a_{10,4} & a_{10,5} & a_{10,6} & a_{10,7} & a_{10,8} & a_{10,9} & a_{10,10} & a_{10,11} & a_{10,12} \\
  a_{11,1} & a_{11,2} & a_{11,3} & a_{11,4} & a_{11,5} & a_{11,6} & a_{11,7} & a_{11,8} & a_{11,9} & a_{11,10} & a_{11,11} & a_{11,12} \\
  a_{12,1} & a_{12,2} & a_{12,3} & a_{12,4} & a_{12,5} & a_{12,6} & a_{12,7} & a_{12,8} & a_{12,9} & a_{12,10} & a_{12,11} & a_{12,12}
\end{bmatrix}
\begin{bmatrix}
  V \\
  \omega \\
  J_1 \\
  J_2 \\
  J_3 \\
  J_4 \\
  J_5 \\
  J_6 \\
  J_7 \\
  J_8 \\
  J_9 \\
  J_{10} \\
  J_{11} \\
  J_{12}
\end{bmatrix}
= \begin{bmatrix}
  B_v \\
  B_\nu \\
  B_\lambda \\
  B_\mu \\
  B_\iota \\
  B_\kappa \\
  B_\theta \\
  B_\phi \\
  B_\rho \\
  B_\sigma \\
  B_\tau \\
  B_\chi \\
  B_\psi \\
  B_\Omega
\end{bmatrix}
(5.2-28)

The global system can be solved in a number of ways. The most straightforward would be to use a standard simultaneous equation solver based on Gaussian elimination or LU decomposition. This is not the most efficient method of solving the system, as it requires the entire matrix to be solved even if the system is only sparsely populated or banded as this system is. A sparse solver that detects the structure of the matrix to be solved and then only solves the non-zero elements is employed. This method is very efficient compared to the standard Gaussian based solvers. In tests carried out it had been found to be at least four times faster but in some cases approximately ten times faster.

5.2.6 Verification of the cavity ‘element’.

The cavity ‘element’ can be verified using a set of simple cases for which the solutions are known, either exactly or in terms of their trend.
CHAPTER 5 A SIMPLIFIED FINITE ELEMENT SCHEME FOR THE MODELLING OF MULTIPLE CAVITIES
ON A SINGLE GRAIN BOUNDARY.

Test 1. Cavity Ripening.

The system consisted of one small cavity and one large one (Figure 71). The ends of the system were sealed and relative motion, both separation and rotation between the grains was prevented. Under these conditions the chemical potential is higher at the larger cavity and the matter should flow away from the larger cavity towards the smaller cavity. The end result should be that the smaller cavity shrinks by the same amount as the larger one grows.

The following data was used for this test: \( R_1 = 3.5 \text{ mm}, R_2 = 0.5 \text{ mm}, \Psi = 150^\circ, M_s = 1.0 \text{ mm}^4 \text{s kg}^{-1}, M_{gb} = 3 \times 10^{-4} \text{ mm}^4 \text{s kg}^{-1}, L = 40 \text{ mm} \). The larger cavity was set to be 7 times bigger than the smaller one, with both cavities using a dihedral angle of 150°. The surface mobility was set to be approximately 3000 times faster than the grain boundary mobility to ensure the cavities stayed spherical for this test. Under these conditions the model produced the following values of rate of change of area, \( \dot{A} \), at the initial time step:

\[
\dot{A}_{\text{large}} = 0.00010624 \text{ mm}^2 \text{s}^{-1} \text{ (Large cavity growing)}
\]

\[
\dot{A}_{\text{small}} = -0.00010624 \text{ mm}^2 \text{s}^{-1} \text{ (Small cavity shrinking)}
\]

Thus, the model has proved mass is conserved.

Test 2. Cavity ‘shifting’ due to applied rotation.

The purpose of this test was to ensure that the mechanism for the cavities to ‘shift’ up and down the grain boundary was working correctly. This test used equal sized cavities of
CHAPTER 5 A SIMPLIFIED FINITE ELEMENT SCHEME FOR THE MODELLING OF MULTIPLE CAVITIES ON A SINGLE GRAIN BOUNDARY.

radius $R = 1.5$ mm. The other parameter values used were $\Psi = 150^\circ$, $M_s = 1.0 \text{ mm}^4 s^{-1}$, $M_{gb} = 3 \times 10^{-4} \text{ mm}^4 s^{-1}$, $L = 40$ mm and $\omega = 10$ rad s$^{-1}$. The ends were again sealed and the grains were prevented from separating ($V = 0$). This time a positive rotation (anticlockwise) was applied. The cavities should move to the right of the system as the material was being ‘squeezed’ from the right hand side to the left. This meant that there should be a positive value for each $\dot{x}_c$. Upon running the model the following results were produced:

$$\dot{x}_{c1} = 3.1314 \times 10^2 \text{ mm s}^{-1} \quad \text{(Left cavity moving to the right)}$$
$$\dot{x}_{c2} = 3.1314 \times 10^2 \text{ mm s}^{-1} \quad \text{(Right cavity moving to the right)}$$

The model results agreed with the expected trend and when the direction of the rotation was reversed the direction of travel of the cavities was also reversed.

**Test 3. Reduction of the simplified finite element model to the single cavity model.**

This test was designed to reduce the simplified finite element model to the single cavity model in chapter 4. This system used two identical cavities with $R = 1.5$ mm and $\Psi = 150^\circ$ that were equally spaced on the grain boundary. The other parameter values were $M_s = 1.0 \text{ mm}^4 s^{-1}$, $M_{gb} = 3 \times 10^{-4} \text{ mm}^4 s^{-1}$, $L = 40$ mm and $\omega = 0$. The ends of the system were sealed as before and there was an applied stress of 25 MPa acting at the centre of the system. The rate of growth of each cavity should be identical and should also agree with that of the 2 degree of freedom model.

<table>
<thead>
<tr>
<th>Simplified finite element model results</th>
<th>2 degree of freedom model results</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V = 1.14 \text{ mm s}^{-1}$</td>
<td>$V = 1.14 \text{ mm s}^{-1}$</td>
</tr>
<tr>
<td>$\dot{R}_1 = 1.497 \times 10^1 \text{ mm s}^{-1}$</td>
<td>$\dot{R} = 1.497 \times 10^1 \text{ mm s}^{-1}$</td>
</tr>
<tr>
<td>$\dot{R}_2 = 1.497 \times 10^1 \text{ mm s}^{-1}$</td>
<td>$\dot{\Psi} = -1.80 \times 10^1 \text{ rad s}^{-1}$</td>
</tr>
<tr>
<td>$\dot{\Psi}_1 = -1.80 \times 10^1 \text{ rad s}^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\dot{\Psi}_2 = -1.80 \times 10^1 \text{ rad s}^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>
Table 5-1 shows the results obtained. It can be seen from Table 5-1 that the simplified finite element model gives the same results as the model given in chapter 4 under the same conditions. The table also shows that the growth rates of the two cavities are the same, and thus agrees with the predictions. As a further test of the simplified finite element model, various other stress levels were applied and there was complete agreement with the model in chapter 4 for all of the cases tested.

**Test 4. Testing of direction of flux flow and cavity shrinkage.**

In this test the grain boundary flux is supplied from one end of the system with the other end sealed.

![Figure 72. System layout for flux flow test.](image)

The relative motions of the grains are prevented (Figure 72). In this case the rate of change of cavity area should be the same as the supplied grain boundary flux flow rate.

The following system parameters were used: $R = 1.5$ mm, $\Psi' = 150^\circ$, $M_g = 1.0$ mm$^4$ s kg$^{-1}$, $M_{gb} = 3 \times 10^{-4}$ mm$^4$ s kg$^{-1}$, $L = 10$ mm, $V = 0$ and $\omega = 0$. In this test there was an applied flux of $0.002339$ s$^{-1}$ mm$^{-2}$ being pumped in from the left. If the model is correct the cavity should shrink at a rate of $-0.002339$ mm$^2$ s$^{-1}$. The results are shown in Table 5-2.

Table 5-2 shows that the cavity does shrink at the same rate as the material being pumped in to the system. The case was also tested where material was sucked out of the system.
In this case the cavity should grow by the same rate as the material being drawn out. The simplified finite element model correctly simulated this test as well.

Table 5-2. Results from the flux flow test.

<table>
<thead>
<tr>
<th>Simplified finite element model results</th>
<th>Rate of change of Cavity Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J^- = 0.002339 \text{ s}^{-1} \text{ mm}^2$</td>
<td>$A_{red} = -0.002339 \text{ mm}^2 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\hat{R} = -0.0018 \text{ mm} \text{ s}^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\hat{\Psi} = 0.002161 \text{ rad} \text{ s}^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>

**Test 5. Testing effect of node position on solution.**

The nodal position between the cavity elements is arbitrary and should have no effect on the outcome of the simplified finite element model. The purpose of this test was to check that this is indeed the case.

Table 5-3. Results from node position test.

<table>
<thead>
<tr>
<th>Nodal Dosition</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$</td>
<td>$-3.12 \times 10^2$</td>
<td>$-3.12 \times 10^2$</td>
</tr>
<tr>
<td>$\hat{R}$</td>
<td>$-4.11 \times 10^1$</td>
<td>$-4.11 \times 10^1$</td>
</tr>
<tr>
<td>$\hat{\Psi}$</td>
<td>$4.94 \times 10^1$</td>
<td>$4.94 \times 10^1$</td>
</tr>
<tr>
<td>$J_0^2$</td>
<td>0</td>
<td>$-1.56 \times 10^1$</td>
</tr>
</tbody>
</table>

This test uses a two-cavity system that is symmetrical and changes the position of the central node, so that it is no longer midway between the elements. There is no applied stress or rotation were ($\sigma = 0$ and $\omega = 0$), but the ends are sealed as before. The system parameters used for this test were $R = 1.5 \text{ mm}$, $\Psi = 150^\circ$, $M_s = 1.0 \text{ mm}^4 \text{ s kg}^{-1}$, $M_{gs} = 3.0 \times 10^4 \text{ mm}^4 \text{ s kg}^{-1}$, $L = 40 \text{ mm}$. The initial position of the node was located at $x = 20 \text{ mm}$ (in the centre of the system). This was then changed to $x = 15 \text{ mm}$ (to the left-hand side of the system). The solution should remain unchanged except for the fact that there should now be a flux flowing across the middle node, whereas before it would have been very small.
Table 5-3 shows that the systems remains unchanged, with the cavities remaining identical in their solution. The only difference is the value of the flux at the new node position. It can be seen that in nodal position 1 where the system is symmetrical the flux across the node is zero. However, when the node has been moved to nodal position 2 it can be seen that there is now a flux at the node equal in magnitude to the rate of change of cavity radius.
5.3 Cavity coalescence.

When two cavities grow close to each other, they coalesce to form a bigger cavity as shown in Figure 73.

![Diagram of cavity coalescence](image)

**Figure 73. Example of observed cavity coalescence.**

It is possible to simulate the coalescence using the full finite element method by Pan et al., (1997). Under the conditions that the simplified 2 degree of freedom model can adequately describe the cavity growth, it was shown that the detailed coalescence process has little effect on the growth behaviour of the total damage area, $L_d$, indicated in Figure 73. The transformation from (a) to (c) can be considered instantaneous, (Kodalatis, 1999). In this work it is assumed that once the distance between the tips of the two cavities reaches a critical value, $L_{cr}$, as shown in Figure 73(a), the two cavities can be instantaneously replaced by a single larger cavity. It is assumed that the damage area of the large cavity is the same as the total damage area of the two smaller cavities, as shown in Figure 74.

![Diagram of cavity coalescence](image)

**Figure 74. Method of cavity coalescence.**
The total volume of the cavities is therefore not conserved during coalescence. It is further assumed that the dihedral angle of the new cavity is the average of the dihedral angles of the two smaller cavities.

\[ \Psi_{\text{new}} = \frac{\Psi_1 + \Psi_2}{2} \]  

(5.3-1)

Since the new length of the coalesced cavity is given as the sum of the original two cavity lengths \((l_1 \text{ and } l_2)\), the value of the radius of the new cavity can be calculated as:

\[ R_{\text{new}} = \frac{l_1 + l_2}{2 \sin \left( \frac{\Psi_{\text{new}}}{2} \right)} \]  

(5.3-2)

The new position of the centre of the coalesced cavity has to be calculated in order for it to be placed on the grain boundary. The position of the new cavity centre \((x_c)\) is given by:

\[ x_{\text{new}} = \frac{(x_{c_1} - hcl_1) + (x_{c_2} + hcl_2)}{2} \]  

(5.3-3)

The method for cavity coalescence has been described above but not the criterion for it to occur. The main factor in deciding whether two cavities are going to coalesce is the critical size of the distance between them as shown in Figure 73(a). Above a certain distance the cavities will continue to grow separately, below that distance and the cavities will coalesce together. Deciding the value of this ‘critical’ length is an arbitrary choice, but it should be consistent with the other parameters such as cavity size and grain boundary length. In this work, the critical length is taken as a quarter of a newly nucleated cavity half-length \((\text{Equation (5.3-4)})\). The nucleation of cavities is discussed in detail in section 5.4.

\[ l_{\text{crit}} = 0.25 \times \left( R_{\text{crit}} \sin \left( \frac{\Psi_{\text{new}}}{2} \right) \right) \]  

(5.3-4)

This is purely an empirical choice.
The final operation carried out is the re-ordering and re-meshing of the nodes after a cavity has been coalesced. This is due to the removal of one cavity ‘element’ as it is combined into another. The nodes, which are represented by the ends of each element have to be re-positioned so that they fall midway between adjacent cavities, this ensures that the grain boundary is the same length each side of the node.

![Diagram of new position of node](image)

**Figure 75. Re-meshing nodes after coalescence.**

Using Figure 75 the following expression is derived giving the new nodal position so that it is midway between the two cavity tips:

\[
\text{new node} = \frac{\left( x_{c1} + R_1 \sin \frac{\psi_1}{2} \right) + \left( x_{c2} - R_2 \sin \frac{\psi_2}{2} \right)}{2} \tag{5.3-5}
\]

Multiple coalescence can occur at the same timestep, these can be consecutive cavities or they can be at various positions on the grain boundary. The computer program has been designed to be able to simulate this occurrence and has been tested using sample cases.

Although cavity coalescence could occur throughout the lifetime of the creep damage process, it only occurs frequently in the very late stages of the creep life. In this late stage, damage accelerates very rapidly, hence the details in the coalescence model has little effect on the predicted total creep life.
5.4 Cavity Nucleation.

The random nucleation of new cavities is an important mechanism that has been incorporated into the simplified finite element model. There are two main approaches that can be taken regarding the type of nucleation model used; these are thermodynamic based models and empirical based models. Yoo and Trinkaus, (1983) conclude that at high temperatures the grain boundary cohesive strength is never exceeded by the local stresses. The thermal models predict nucleation to be possible only at applied stresses that are approximately 100 times higher than those usually present in engineering applications (Dyson, 1983). Hence these models do not predict nucleation under the present conditions and the empirically derived nucleation law from Davanas and Solomon, (1990), was used in this work. As discussed in the literature review, the nucleation of cavities is generally found to be continuous and linear with the time-dependent strain, Needham and Gladman, (1980), Page and Lankford, (1983). Needham and Gladman, (1980), suggest that for creep of type 347 stainless steel:

\[
J = B \dot{\varepsilon}
\]

(5.4-1)

where \( J \) = nucleation rate (cavities per unit area and time), \( \dot{\varepsilon} \) = time dependent creep strain rate (\( s^{-1} \)) and \( B \) is assumed to be a nucleation rate constant.

The total plastic strain rate, \( \dot{\varepsilon} \), can be related to the remote stress \( \sigma_r \) by:

\[
\dot{\varepsilon} = A \frac{\sigma_r^n}{d^m}
\]

(5.4-2)

in which \( A \) is a material constant which depends on the operating temperature, \( d \) is the grain size, \( n \) and \( m \) are material constants which depend on the mechanism by which the surrounding matrix deforms.

Combining (5.4-1) and (5.4-2) we have:
The parameter $B$, is not well known for creep experiments and was determined by a trial and error method which is discussed further in the results section.

The size of the newly nucleated cavities is determined by the applied stress ($\sigma_\infty$) and the free surface energy ($\gamma_s$). The radius of the cavity must be above a ‘critical’ value ($R_{\text{crit}}$), for the cavity to grow and we have:

$$R_{\text{crit}} = \frac{\gamma_s}{\sigma_\infty}$$  \hspace{1cm} (5.4-4)

The nucleation site is generally considered as random. Hence, a random number generator chooses the position of the new cavities on the grain boundary. There are many different random number generators available. The position of the nucleated cavities is not absolutely critical, and only need to be placed at different positions at different times, as opposed to a fixed layout. The generator used is reference by Press et al., (1994), and has a long period (>2x10^{18}) and is by L’Ecuyer with a Bays-Durham shuffle. It returns a uniform deviate between 0.0 and 1.0 and is initialised using a negative integer.

When the nucleation model given by (5.4-3) was employed in the computer model using the values quoted by Davanas and Solomon, (1990), it was found to produce nucleation dominated damage evolution. The material parameters were adjusted to attempt to compensate for this however, the nucleation rate was found to be too high and was preventing the existing cavities from growing and interacting with one another. For this reason (5.4-3) was not used in the final computer model, instead a nucleation rate was chosen which would produce approximately 200 cavities during the lifetime of the system. This was reasonable number of cavities and allowed the interaction and coalescence of cavities to be simulated.
CHAPTER 5 A SIMPLIFIED FINITE ELEMENT SCHEME FOR THE MODELLING OF MULTIPLE CAVITIES
ON A SINGLE GRAIN BOUNDARY.

5.5 Calculation of local grain boundary stress.

Once all the degrees of freedom are solved from equation (5.2-28), the local grain boundary stress can be determined from these degrees of freedom. In this section, the procedure used to calculate the stress is described.

5.5.1 Sign convention for curvature.

If we have a surface as shown below in Figure 76., then the flux will flow in the direction shown. The sign conventions for the curvatures, \( \kappa \), and chemical potentials, \( \mu \), shown in Figure 76.

![Figure 76. Direction of flux flow on a free surface.](image)

The above surface will evolve to a flat surface, at which point there will be no chemical potential difference anywhere along the surface.

5.5.2 Chemical potential along the free surface.

To determine the grain boundary stress, the chemical potential at the cavity tip has to be found first. The method used to derive the chemical potential expressions is based on the so-called 'weak' solution. In this work an arc with a radius \( R \) is used to approximate the cavity surface. We therefore assume a constant curvature for the arc.
CHAPTER 5 A SIMPLIFIED FINITE ELEMENT SCHEME FOR THE MODELLING OF MULTIPLE CAVITIES ON A SINGLE GRAIN BOUNDARY.

The chemical potential is related to the curvature by:

\[ \mu = -\gamma_s \Omega k \]  \hspace{1cm} (5.5-1)

where \( \Omega \) is the atomic volume. The surface flux \( J_s \) is related to the chemical potential by the expression:

\[ J_s = -\frac{\partial \mu}{\partial s} \]  \hspace{1cm} (5.5-2)

and from (5.5-2) it would seem that the constant curvature of an arc would not produce a flux. The use of the ‘weak’ solution overcomes this. In the weak solution, the relationship between the chemical potential and the curvature given by (5.5-1) is ‘released’, and does not have to be satisfied when using the variational principle. It can be shown that the minimisation of \( \Pi \) satisfies the relationship given by (5.5-1) in the variational sense. This approach is analogous to the use of a linear displacement field in a classical finite element model. For example, when using triangular elements one can assume a constant strain is present which leads to a constant stress across the element. This is not possible in reality, as there would be step changes from element to element and there would not be a force balance. However, the finite element method ensures that there is a global force balance, and thus satisfies the requirements for the problem to be solved. Using the variational principle we obtain the functional \( \Pi \), which is a function of the surface flux \( J_s \), which in turn is written in terms of the degrees of freedom. Upon minimisation the functional yields an expression that can be easily solved, giving a value for the surface flux \( J_s \) (5.5-17). This can then be used to calculate the chemical potential at any point on the free surface of the cavity in terms of the local co-ordinate \( (s) \). The full expression for surface flux is given by equation (5.5-3).

\[ J_s = -\frac{D_s \delta_s \partial \mu}{kT} \partial_s \]  \hspace{1cm} (5.5-3)

Where \( D_s \) is the surface diffusivity, \( \delta_s \) is the effective thickness of the diffusion layer, \( k \) is Boltzmann’s constant and \( T \) is temperature. For later convenience, we re-write (5.5-3) as:
which leads to

\[
\bar{\mu}_s = -\frac{1}{M_s} \int J_s \, ds + \mu_0
\]  

(5.5-4)

in which \( M_s = \frac{D_s \delta_s \Omega}{kT} \), \( \bar{\mu} = \frac{\mu}{\Omega} \), \( \Omega \) is the atomic volume and \( \mu_0 \) is the constant of integration which is simply the chemical potential at \( s=0 \), and needs to be determined. Equation (5.5-4) can be integrated over the entire free surface to give the average chemical potential over the free surface.

\[
\bar{\mu}_{s, \text{average}} = \frac{1}{L} \int_{-\Psi/2}^{\Psi/2} \bar{\mu}_s R \, d\theta
\]  

(5.5-5)

in which \( L \) is the total length of the free surface.

Figure 77 shows the parameters used in the calculation of the local stress. \( \theta \) gives the local angle of the free surface and \( s \) gives the local length of the free surface. Because an arc approximates the free surface, and the average curvature is \( 1/R \), therefore, the average chemical potential for the surface must be \(-\gamma_s / R\).

\[
\frac{1}{L} \int_{-\Psi/2}^{\Psi/2} \bar{\mu}_s R \, d\theta = -\frac{\gamma_s}{R}
\]  

(5.5-6)
This provides the conditions needed to determine \( \mu_0 \) in Equation (5.5-4). By substituting the expression of \( J_s \) in section 5.2.4 into (5.5-4) and using (5.5-6), we obtain:

\[
\mu_0 = \frac{1}{R^2} \left\{ -\frac{\gamma_s L}{R} + \frac{R^2}{M_s} \left[ \frac{RR^3}{24} + 2RR\cos \frac{\Psi}{2} \left( \frac{\psi}{2} - \frac{\psi}{2} \right) + R^2 \sin \frac{\Psi}{2} \left[ \frac{\psi}{2} - \sin \frac{\psi}{2} \right] \right] \right\}
\]

(5.5-7)

Equation (5.2-17) is then inserted into the expression for \( \bar{\mu}_s \) in equation (5.5-4) and integrated from \((0, \theta)\), which gives a general expression for \( \bar{\mu}_s \) in terms of \( \theta \):

\[
\bar{\mu}_s = -\frac{1}{M_s} \int_0^\theta J_s R \theta + \bar{\mu}_0
\]

(5.5-8)

We then enter the value of \( \theta \) at the cavity tip as that is the position where chemical potential is required, this gives us an expression for the chemical potential at the tip \( \bar{\mu}_{tip} \):

\[
\bar{\mu}_{tip} = -\frac{R}{M_s} \left[ RR \left( \frac{\theta^2}{2} + \cos \frac{\Psi}{2} (\cos \theta - 1) \right) + R \xi_c \left( \theta \cos \frac{\Psi}{2} \sin \theta \right) + \frac{\Psi^2}{2} \sin \left( 1 - \cos \theta \right) + J_c^0 \theta \right] + \bar{\mu}_0
\]

(5.5-9)

The expression for \( \mu_0 \) is inserted into equation (5.5-9) and yields the expression for \( \bar{\mu}_{tip} \):

\[
\bar{\mu}_{tip} = \frac{1}{24R^3\Psi M_s} \left[ R^4 \hat{\xi} \Psi^3 + 48R^4 \hat{\xi} \sin \frac{\Psi}{2} \cos \frac{\Psi}{2} - 24R^4 \hat{\xi} \sin^2 \frac{\Psi}{2} - 24\gamma_s LM_s \right.
\]

\[
-12R^4 \hat{\xi} \Psi^2 - 24R^4 \hat{\xi} \cos \frac{\Psi}{2} \cos \theta + 24R^4 \hat{\xi} \xi_c \sin \theta
\]

\[
-24R^4 \Psi \xi_c \cos \frac{\Psi}{2} \theta + 12R^4 \hat{\xi} \Psi \sin \frac{\Psi}{2} \cos \theta - 24R^3 \Psi J_c^0 \theta \left. \right]
\]

(5.5-10)

At the cavity tip, the continuity of the chemical potential requires that:

\[
\mu_{tip} = -\sigma_{tip} \Omega
\]

or

\[
\bar{\mu}_{tip} = -\sigma_{tip}
\]

(5.5-11)
We have now arrived at the expression for the local stress at the cavity tip and this can be used to calculate the local stress at any point on the grain boundary. The derivation is given in Section 5.5.3.

Figure 78. System used for comparison of chemical potential as a function of mobility ratio and applied stress.

Figure 78 shows the type of system considered for the comparison of chemical potential as a function of mobility ratio and applied stress. It is a single cavity system with the radius of the cavity set to value of unity. The normalised chemical potential $\mu / (\mu_s / R)$ will also be unity if the cavity grows in an equilibrium manner. The equilibrium growth can be achieved by a combination of low applied stress and high $M_s / M_{gb}$.

Table 5-4 gives several cases showing how $\mu_{ip}$ varies with different applied stresses and ratios of mobility. It should be noted that the applied stress has been normalised with respect to the sintering stress, with the following values used for the variables: $R = 1$, $\Psi = 150^\circ$ and $L = 3.927$. The values of $\dot{R}$, $\dot{\Psi}$ and $\dot{x_c}$ vary according to the applied conditions and are not listed explicitly.
Table 5-4. Comparison of $\mu_{\text{tip}}$ values as a function of mobility ratio and normalised applied stress.

<table>
<thead>
<tr>
<th>$\mu_{\text{tip}} / (\gamma_s / R)$</th>
<th>$M_s / M_{gb}$</th>
<th>$\sigma_m / (\gamma_s / R)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.97558</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>-1.00005</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>-2.19906</td>
<td>1</td>
<td>50</td>
</tr>
<tr>
<td>-3.42254</td>
<td>1</td>
<td>100</td>
</tr>
<tr>
<td>-13.2104</td>
<td>1</td>
<td>500</td>
</tr>
<tr>
<td>-1.02252</td>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td>-1.0023</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>-1.00027</td>
<td>1000</td>
<td>100</td>
</tr>
<tr>
<td>-1.00007</td>
<td>10000</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 5-4 shows that (5.5-1) gives the expected value of chemical potential if the stress is low or $M_s / M_{gb}$ is high, and gives higher values of the chemical potential if the growth is not equilibrium. The latter result is expected, since non-equilibrium growth leads to higher curvature at the cavity tip.
5.5.3 Local stress along the grain boundary.

The local stress at any point along the grain boundary can now be calculated as we have already calculated the stress at the cavity tip. The value of $\sigma_{gb}$ is used as a boundary condition in the derivation of the local stress expression. Figure 79 shows the typical system that is being dealt with in the cavity model. The important co-ordinates and lengths are shown, as well as the applied stress.

![Figure 79. Layout of typical cavity system.](image)

The system has now been defined and the governing equations for flux are shown below:

\[
\frac{\partial J_{gb}}{\partial s} + V_{gb} = 0 \quad (5.5-12)
\]

\[
J_{gb} = M_{gb} \frac{\partial \sigma}{\partial s} \quad (5.5-13)
\]

Combining equations (5.5-12) and (5.5-13) we obtain:

\[
\sigma = \frac{1}{M_{gb}} \left[ \frac{V_{gb}s^2}{2} + J_0s \right] + C \quad (5.5-14)
\]

in which $J_0$ is the grain boundary flux across the nodal point of the cavity element, and $C$ is an integration constant which can be determined by either of the two end conditions at the cavity tips.
\[ \sigma = \sigma_{\text{tip}}, \quad s = \frac{1}{2} \]
\[ \sigma = \sigma_{\text{tip}^*}, \quad s = -\frac{1}{2} \]

where \( l \) is the total length of the grain boundary. \( \sigma_{\text{tip}} \) and \( \sigma_{\text{tip}^*} \) are calculated using Equation (5.5-10). If the solutions for the system are consistent, then the values of \( C \) obtained from the two end conditions should be the same. This provides us with a further confirmation of the entire procedure discussed above. The test system was a two-cavity system with radii of 1.0 mm and 1.6 mm respectively, dihedral angle of 150° and total system length of 40 mm. There was an applied stress of 10 MPa and the system was prevented from rotating. The results at \( t = 0 \) s from the model are shown in Table 5-5.

Table 5-5. Results from model for two-cavity system.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Left cavity</th>
<th>Right Cavity</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{R} ) (mm s(^{-1}))</td>
<td>8.169052</td>
<td>4.95739</td>
</tr>
<tr>
<td>( \dot{\psi} ) (rad s(^{-1}))</td>
<td>-14.74349</td>
<td>-5.591995</td>
</tr>
<tr>
<td>( \dot{x}_c ) (mm s(^{-1}))</td>
<td>(-5.485715\times10^2)</td>
<td>(-0.034286)</td>
</tr>
<tr>
<td>( J_x^0 ) (mm(^2) s(^{-1}))</td>
<td>(-3.21187\times10^{-2})</td>
<td>(-3.21187\times10^{-2})</td>
</tr>
<tr>
<td>( J_0 ) (mm(^2) s(^{-1}))</td>
<td>(-1.284752\times10^{-1})</td>
<td>(-1.284752\times10^{-1})</td>
</tr>
<tr>
<td>( \mu_{\text{tip}} ) (N mm)</td>
<td>(-1.23381)</td>
<td>(-1.01226)</td>
</tr>
<tr>
<td>( s ) (mm)</td>
<td>(-9.03407)</td>
<td>(8.45452)</td>
</tr>
<tr>
<td>( V ) (mm s(^{-1}))</td>
<td>(3.996403\times10^{-1})</td>
<td>(3.996403\times10^{-1})</td>
</tr>
</tbody>
</table>

Using the values in Table 5-5 and equation (5.5-14) the value of \( C \) was calculated for the left and right hand sides of the system. The results are shown in Table 5-6.

Table 5-6. Values of integration constants.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Left cavity</th>
<th>Right Cavity</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C )</td>
<td>16.381</td>
<td>16.381</td>
</tr>
<tr>
<td>( C )</td>
<td>16.401</td>
<td>16.401</td>
</tr>
</tbody>
</table>
It can be seen from Table 5-6 that the constants are the same for the left and right sides, so we now average them and form a new constant \( \bar{C} \), which is given below:

\[
\bar{C} = \left[ \frac{\sigma_{\text{tip}} + \sigma_{\text{tip}}}{2} \right] + \frac{V_{gb} I^2}{8 M_{gb}}
\]  

(5.5-15)

Equation (5.5-15) is inserted into equation (5.5-14) to give the final expression for the local stress at any point on the grain boundary:

\[
\sigma = \frac{1}{M_{gb}} \left[ -\frac{V_{gb} S^2}{2} + J \right] + \left[ \frac{\sigma_{\text{tip}} + \sigma_{\text{tip}}}{2} \right] + \frac{V_{gb} I^2}{8 M_{gb}}
\]  

(5.5-16)

As a final means of testing the accuracy of equation (5.5-16), the force balance:

\[
\sigma_\infty L_{\text{Total}} - \gamma_s \sin\left(\frac{\Psi}{2}\right) = \int_0^l \sigma dx
\]  

(5.5-17)

is checked by inserting (5.5-16) into the above integration, here \( L_{\text{Total}} = \) Total length of the system, \( l = \) length of grain boundary, \( \sigma_\infty = \) applied stress.

<table>
<thead>
<tr>
<th>( \frac{M_s}{M_{gb}} )</th>
<th>( \sigma_\infty L_{\text{Total}} )</th>
<th>( \int_0^l \sigma_{\text{local}} dx + \gamma_s \sin\left(\frac{\Psi}{2}\right) )</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.001125</td>
<td>( \infty )</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>9.999925</td>
<td>0.00075</td>
</tr>
<tr>
<td>1</td>
<td>500</td>
<td>499.9413</td>
<td>0.0117</td>
</tr>
<tr>
<td>1</td>
<td>1000</td>
<td>999.8818</td>
<td>0.0118</td>
</tr>
<tr>
<td>1</td>
<td>5000</td>
<td>4999.403</td>
<td>0.012</td>
</tr>
<tr>
<td>10</td>
<td>1000</td>
<td>999.8793</td>
<td>0.0121</td>
</tr>
<tr>
<td>100</td>
<td>1000</td>
<td>999.8790</td>
<td>0.0121</td>
</tr>
<tr>
<td>1000</td>
<td>1000</td>
<td>999.8789</td>
<td>0.0121</td>
</tr>
<tr>
<td>10000</td>
<td>1000</td>
<td>999.8790</td>
<td>0.0121</td>
</tr>
</tbody>
</table>
The results from the different applied stresses are shown in Table 5-7. The values for the system parameters are the same as were used in the production of the results shown in Table 5.5 with $L_{\text{f toll}} = 10$ mm. It can be seen that the force balance is very satisfactory indeed.
5.6 Flowchart for computer program.

The main operation of the computer program is described using the flow chart below, as it clearly demonstrates how all the mechanisms are incorporated into the model.
CHAPTER 5 A SIMPLIFIED FINITE ELEMENT SCHEME FOR THE MODELLING OF MULTIPLE CAVITIES ON A SINGLE GRAIN BOUNDARY.

YES Another element?

Determine timestep size and critical length for coalescence

Update variables using explicit time integration scheme

Check for cavities that are closer together than the critical length and coalesce them, conserving total damage

NO Nucleation time reached?

YES Generate random number for position on grain boundary of new cavity

Scan system for valid segments for nucleation. Determine the random position for nucleation of cavity

Nucleate cavity on grain boundary

Add a new node for the new cavity and re-mesh the system ensuring there are no negative lengths

Re-order the node for the system ensuring they are midway between cavities and correctly stored

Write results to file if output frequency has been reached

YES Another timestep?

End

NO
The rate equations are solved using explicit time integration as described in Section 4.3.4. The size of the timestep is controlled using the same method as described in Section 4.3.5. The size of the controlling value (ALPHA) was again determined by trial and error. The value of ALPHA was found to be quite critical in determining whether the nucleated cavities would grow or shrink.
5.7 Conclusions.

The simplified finite element model can simulate a number of different cavity growth scenarios. It can model a single cavity on a grain boundary with no nucleation, or it can model a large number of cavities with continuing nucleation and coalescence throughout the lifetime until rupture occurs. Cavities can also be placed on the grain boundary before the simulation begins. This allows the modelling of pre-existing damage such as a large 'crack-like' cavity. The nucleation rate can be set manually or calculated based on the applied stress and other material parameters entered as shown in section 5.4. The load can be applied at any position on the grain boundary allowing for a centrally applied load or an off-centred load. The cavities are free to 'shift' up and down the grain boundary depending on the applied conditions. The maximum number of cavities that can be modelled is only limited by the system memory on which the program is running.

The simplified finite element model has been validated using a series of simple tests and has been shown to return the expected results. This new model is used extensively in later chapters to simulate the evolution of multiple cavities on a single grain boundary.

The computer program can output a variety of different results to a file. 'Switches' in the input data file control the types of results required. One of the result files contains the time, damage fraction of the system, separation velocity and number of elements. The damage fraction can be used to plot the evolution of the system. The separation velocity can be used as a means of comparison with other models. A separate file contains the entire data for the system for a given multiple of the output frequency. This allows the entire history of every cavity 'element' on the grain boundary to be plotted, however it can be a very large file and can slow the program down whilst it is writing to disk. The final file has all the data required to graphically plot the evolution of the system. This data was formatted so that a separate program written by the author could read it in. This program plots the cavities on the screen as the system evolves. This allows the user to visualise what is happening on the grain boundary and 'see' the formation of damage on the grain boundary.

6.1 Introduction.

The model used by Nguyen et al. (1998) is fundamentally different from the other models previously discussed as it uses a ‘smeared-out’ approach to model the cavities as opposed to the discrete distribution. The microstructural model incorporates what is called a ‘process window’ by the authors, around the tip of the crack. This contains a large number of grains that are represented discretely by so-called ‘grain elements’. For computational reasons, each grain is represented by a single ‘grain element’. The grain elements are connected by grain boundary elements that account for the fracture mechanisms such as the nucleation of grain boundary cavities, their growth by grain boundary diffusion and by creep of the surrounding material, and their final coalescence leading to micro-cracks. The ‘smeared-out’ model is not yet justified. By comparing the predictions of the ‘smeared-out’ model with those of the discrete simplified finite element model presented in the previous chapter, the validity of the ‘smeared-out’ model can be investigated. This is the focus of the current chapter.

6.2 The ‘smeared-out’ model.

The model by Nguyen et al. (1998) uses a ‘smeared-out’ approach to model the cavities that are present on a grain boundary.

![Spherical cavity on grain boundary](image)

Figure 80. Spherical cavity on grain boundary.
Here, the ‘smeared-out’ model is first briefly introduced for a three-dimensional cavity, then, a two-dimensional version is derived in order to compare with the simplified finite element model, (which is two-dimensional). Figure 80 shows a single 3 dimensional cavity present on a grain boundary.

The representative unit associated with the cavity is assumed to be a circular area with radius \( b \). As the cavity grows, its material is assumed to be uniformly distributed in the circular area, hence we have:

\[
\delta_c \times \pi b^2 = V
\]  

(6.2-1)

Here \( \delta_c \) is the ‘thickness’ of the material inserted into the grain boundary as shown in Figure 81, and \( V \) is the volume of the cavity. Differentiating both sides of (6.2-1), we have:

\[
\delta_c = \frac{\dot{V}}{\pi b^2} - \frac{2V}{\pi b^2} \frac{b}{b}
\]  

(6.2-2)

In the case of two dimensional cylindrical cavities, we have:

\[
\delta_c \times 2b = A
\]  

(6.2-3)

in which \( A \) is the area of the two dimensional cavity. Differentiating (6.2-3) we have:

\[
\delta_c = \frac{\dot{A}}{2b} - \frac{A}{2b^2} \frac{b}{b}
\]  

(6.2-4)
Hence, $\dot{\delta}_c$ is in fact the grain boundary separation velocity $V$, which has been discussed in previous chapters.

It can be seen from (6.2-4) that the rate of change of thickness is composed of two components: a) the cavity growth component given by the first term and, b) the nucleation component in the form of the rate of change of cavity spacing. In this model the nucleation is a continuous rate as opposed to being a step change in damage when a new cavity is placed on the grain boundary.

For a two dimensional cavity, we have:

$$A = R^2(\Psi - \sin \Psi) \quad (6.2-5)$$

and the cavity growth rate can be calculated as:

$$A = 2R\dot{R}(\Psi - \sin \Psi) \quad (6.2-6)$$

Considering a grain boundary of length $L$, along which $N$ cylindrical cavities are uniformly distributed, as shown in Figure 82.

![Figure 82. Assumption of long cylindrical cavities on a grain boundary.](image)

We have:

$$2b = \frac{L}{N} \quad (6.2-7)$$

where $2b$ is the spacing between the cavities.
Differentiating equation (6.2-7) we arrive at an expression for the rate of change of cavity spacing:

\[ \dot{b} = -2b^2 \frac{\dot{N}}{L} \quad (6.2-8) \]

Now inserting (6.2-5), (6.2-6), (6.2-7) and (6.2-8) into (6.2-4) we obtain:

\[ V = \dot{\delta}_c = \frac{R\dot{R}(\Psi - \sin \Psi)}{b} + \frac{R^2 (\Psi - \sin \Psi)}{L} \dot{N} \quad (6.2-9) \]

A variety of different expressions for \( \dot{R} \) and \( \dot{N} \) can be used together with (6.2-9) depending on the considered mechanism for cavity growth and the assumed nucleation model. The purpose of this model is to compare the 'smeared-out' approach with the simplified finite element model. It is therefore consistent to use the rate equation derived in section 4.4.1, i.e.

\[
\dot{R} = \left( \sigma_{\infty} R (\Psi - \sin \Psi) + \gamma_{gs} \sin \left( \frac{2\Psi_e}{2} \right) - \gamma_R \Psi_e - \frac{\gamma_s \sin \left( \frac{2\Psi_e}{2} \right) (\Psi_e - \sin \Psi_e) \dot{R}}{L_0} \right)
\]

\[
\frac{R^2 (\Psi_e - \sin \Psi_e)^2}{3L_0^2} \left( \frac{I^2}{M_{gb}} + \frac{\Psi_e R^2}{M_s} \right)
\]

and the continuous nucleation rate equation discussed in section 5.4, i.e.

\[ \dot{N} = B \dot{\delta} \]

Using the expressions listed above it is also possible to derive an expression for the initial time, \( t_0 \). (6.2-10) gives this as:

\[ t_0 = \frac{1}{\dot{N}} \quad (6.2-10) \]

The purpose of the initial time is to show that at time \( t = t_0 \) the value of \( N = 1 \). This shows that there is one cavity present on the grain boundary when the simulation is started. If this were not the case there would be no damage on the grain boundary.
6.3 Damage due to nucleation in the 'smeared-out' model.

Obviously, the 'smeared-out' model is unable to simulate the interactions between the cavities. Furthermore, the size of a newly nucleated cavity has to be the same as the existing cavity size at the time at which nucleation occurs. Therefore, the model nucleates larger and larger cavities. In reality the size of the newly nucleated cavities should be very small compared with the characteristic length of the system (grain size for example). This is a major problem for the 'smeared-out' model.

It is possible to evaluate the contribution of the nucleation to the total damage in the model. The method used is shown below:

Over a time interval $dt$, the damage increase due to nucleation is:

$$\frac{d{\text{Damage}}_{\text{nuc}}}{dt} = \frac{N dt \times l(t)}{L} \quad (6.3{-}1)$$

where $l$ is the cavity length at the time of nucleation:

$$l = 2R \sin \frac{\Psi}{2}$$

and $L$ is the total length of the grain boundary. Integrating (6.3-1) we have:

$$\text{Damage}_{\text{nuc}} = \frac{N}{L} \int_0^t l(t) dt \quad (6.3{-}2)$$

As an example, we consider a case of a grain boundary with the following parameters $\sigma_\infty = 10\text{MPa}$, $\Psi = 120^\circ$, $L_T = 0.25\text{mm}$, $R = 2.24 \times 10^{-4}\text{mm}$, with the relative mobility $M_s/M_{gb} = 10$ and a nucleation rate, $N = 4.569 \times 10^4 \text{s}^{-1}$. Figure 83 gives the total damage and the damage due to nucleation predicted by the 'smeared-out' model as a function of time. It can be seen that the contribution from nucleation is as large as 34% approaching the end of the creep life. In reality this contribution should be negligible.
Figure 83. Example of contribution to damage by nucleation.

Figure 84 shows a flow chart detailing the general order of operation for the ‘smeared-out’ model. This shows how the various parameters that were defined in the previous sections are combined to produce the working model.
Set values of initial parameters and initial conditions, (Applied stress, dihedral angle, mobility values, etc)

Calculate initial values of parameters (cavity area, damage etc.)

Write initial values to file

Calculate rate of change of cavity spacing reduction ($\delta$)

Calculate rate of change of cavity radius

Calculate rate of change of cavity area ($\delta a$)

Calculate the rate of change of thickness of the cavity ($\delta t$)

Calculate the timestep size using adaptive method

Update the parameters using explicit method

Write results to file

Has critical damage fraction been reached?

No

Yes

End

Figure 84. Flow chart of operation for ‘smeared-out’ model.
6.4 Results.

As discussed in section 6.3, the major drawback of the 'smeread-out' model is that it exaggerates the contribution from nucleation to the damage growth. This effect is fully demonstrated in this section. The purpose here is to determine the conditions under which the 'smeread-out' model and the simplified finite element model agree.

The two models are expected to agree to a better extent if the nucleation of cavities does not contribute significantly to the damage growth. This condition can be achieved either by increasing the level of the applied remote stress while maintaining the nucleation rate constant, or by decreasing the nucleation rate while keeping the applied stress constant.

6.4.1 Parameters used in computer simulations.

There are several parameters that are used in both the 'smeread-out' and simplified finite element models throughout the simulations that require explanation before the results are presented. Unless otherwise stated the values listed here are used for all the simulations in this chapter. The first parameter is the timestep controlling value \( \alpha \), which is discussed in section 4.3.4. This value was determined empirically for these simulations and \( \alpha = 2 \times 10^{-6} \) was found to give the most acceptable results.

In all the simulations the total length of the system \( L_r \), was set as 0.25 mm. This is a relatively large grain size but the value is taken from Davanas and Solomon, (1990), who used data for copper in their simulations, the complete listing of material data is given in Appendix C.

The final parameter that is common to the simplified finite element and 'smeread-out' models is the size of the nucleating cavity radius \( R \). This was based on the critical radius value with a scaling factor, \( \delta \), to ensure the cavities grew. The nucleating cavity radius is calculated using:

\[
R = \delta \frac{\gamma_s}{\sigma}
\]
where \( \gamma_s = 1.725 \times 10^{-3} \text{ J mm}^{-2} \) and is the surface tension value for copper and \( \sigma \) is the applied stress. The determination of \( \delta \) was empirical and it was found that a value of \( \delta = 1.3 \) was sufficient to ensure the cavities grew. This was the case for all of the simulations except those with an applied stress of 5000 MPa. In this case there were numerical instabilities and the value of \( \delta \) had to be increased from 1.3 to 10 to ensure cavity growth. Although there is no justification for this, it is an unrealistically high applied stress that was analysed to push the model to the extremes and observe the trends produced.

6.4.2 Approaching the growth controlled limit by increasing the applied stress.

**Case 1** \(- M_g = 2.08 \times 10^{-16}, M_{gb} = 2.08 \times 10^{-17}, M_g/M_{gb} = 10.\)

The first simulation used the parameters: \( M_g/M_{gb} = 10 \), Dihedral Angle = 120° and a nucleation rate \( N \) of \( 4.569 \times 10^4 \text{ s}^{-1} \). This nucleation rate was chosen such that approximately 200 cavities are nucleated in the entire creep life of the grain boundary if a stress of \( \sigma_s = 10 \text{ MPa} \) is applied. The stress is then increased to 50, 500 and 5000 MPa to search for its critical value at which the two models agree with each other.

There were four main parameters that were compared to enable conclusions to be drawn about the accuracy of the 'smeared-out' model. These were total damage fraction, separation velocity, cavity spacing and cavity size. The calculations detailed in section 6.3 showing the contribution from nucleation separately were also used to determine the accuracy of the 'smeared-out' model.

The first parameter used in the comparison process was the damage fraction. This gives the amount of grain boundary that has cavities present on it as a fraction of the total length of the grain boundary. Figure 85 shows the damage evolution for Case 1 and Figure 86 shows an enlarged view of the initial region of the graph (highlighted by dotted lines).
This case is designed to show the effects of nucleation by holding the nucleation rate constant. The range of applied stress was varied from 10 MPa, which is a relatively low applied stress up to 5000 MPa, which is a very high and unrealistic stress. This high value of stress was chosen to accentuate the trends and clearly show the decreasing effect of
nucleation. Figure 6 shows a void growth map from Cocks and Ashby, (1982). This shows the dominating mechanism for the growth process in copper at varying stresses and temperatures. If the normalised tensile stresses are calculated based on the applied stresses stated above, the values produced places the model in the area where growth is controlled by surface diffusion. The applied temperatures are also in the correct range as we are operating in the range of $0.2 - 0.8T_{\text{melt}}$. The materials data given in Appendix C shows real material values for the mobility ratio $(M_g/M_{gb})$. It is notoriously difficult to obtain accurate data for diffusion coefficients, and whereas the trend that can be seen in the ratio of mobilities increasing with temperature the absolute values of the ratios cannot be assumed to be accurate. It can be seen that these ratios range from $2.01 \times 10^{-3}$ for copper to $6.48 \times 10^{-4}$ for titanium aluminate. Therefore, the range in which the simulations have been conducted in $(M_g/M_{gb} = 1$ to $M_g/M_{gb} = 100)$, places them in the centre of the actual material data.

Figure 85 shows the damage evolution for the various applied stresses from the simplified finite element and ‘smeared-out’ models. On the x-axis is time in seconds and on the y-axis is damage fraction. The grain boundary was assumed to fail at 80% damage, therefore the simulations were programmed to stop upon reaching a damage fraction of 0.8. It can be seen that, as expected, the higher the applied stress the shorter the lifetime of the material. The nucleation rate was held constant using the value that applies to an applied stress of 10 MPa. The simplified finite element model predicts a longer time to failure than the ‘smeared-out’ model in all but the very high applied stress simulations. This is due to the effect of nucleation in the ‘smeared-out’ model. As the size of nucleated cavities increases during the evolution the damage rate accelerates far quicker than predicted by the simplified finite element model.

It can be seen from Figure 86 that the two models are in very good agreement at the very beginning of the process. This is expected because, at the initial stages the effects of nucleation and cavity interaction have not come in to play, and the ‘smeared-out’ model is able to simulate the majority of the behaviour well. The agreement between the two models in the initial stages of the damage process provides a further confirmation of the computer implementation of the two models. However, the agreement only lasts for a very short period of time.
The percentage differences between rupture times shown in Figure 85 decrease as the applied stress increases. This suggests that cavity growth is becoming the more dominant mechanism in the system. It can also be seen that the length of the linear section of the damage curve reduces as the applied stress increases. This shows that as applied stress is increased cavity growth and coalescence occur at an earlier time in the evolution.

![Figure 87. Separation velocity for 'smeared-out' and simplified finite element models.](image)

Figure 87 shows the separation velocity as a function of time for the different applied stresses. It can be seen that the simplified finite element and 'smeared-out' models only agree well when the applied stress is an unrealistically high value, in this case 5000 MPa. There is quite a good agreement between lines ‘A’ and ‘a’ that represent the simplified finite element model and the ‘smeared-out’ model respectively. However, as the applied stress is reduced the lines tend to diverge and there is a larger difference between lines ‘C’ and ‘c’, especially considering that the x-axis is using a logarithmic scale. Figure 87 reinforces the conclusions drawn from the damage fraction graph, i.e. that the ‘smeared-out’ model only works at unrealistically high stresses. It can be seen that at realistic stress ranges, the ‘smeared-out’ model significantly under-predicts the time for the creep damage to accelerate.
The cavity size and spacing distributions during the damage evolution were also investigated using the results from the simplified finite element model. The cavities were divided into size ‘ranges’ i.e. all the cavities that fell between the range of sizes were counted and tabulated. This gave the frequency of that particular size range. This was repeated over the entire size range of cavities with the result being a complete picture of the size distribution of cavities. This procedure was also carried out for the spacings between the cavities.

The frequency of cavity sizes and spacings was calculated to determine whether there was a pattern in the way the system evolved. The frequencies were plotted in a histogram at three different damage fractions of 25, 40 and 75%, giving three ‘snapshots’ of the system. The y-axis of the histograms represents the number of cavities or spacings, with the x-axis representing the range of values that were used to divide the system up. The results from this operation did not yield any new information, although they did confirm what had been assumed to happen. For this reason only the first case will have the histograms shown as an example, the other cases were examined with much the same conclusions being drawn.

Figure 88 shows the distribution of cavity radii on the left and the distribution of cavity spacing on the right for an applied stress of 50 MPa. For the cavity radii distribution each bar represents a range of $2 \times 10^{-4}$ mm, and for the cavity spacing distribution each bar represents a range of $3 \times 10^{-4}$ mm. There are three damage fractions shown (25, 40 and 75%). The cavity size distribution graphs show that as the damage increases the range of cavity sizes increase. There are two main reasons for this, the first is that as the cavities grow at differing rates depending on their size and position there will become a wider range of sizes. The second reason is the nucleation of new cavities is continuing throughout the lifetime of the simulation. Thus introducing new small cavities that will grow as the system evolves. The cavity spacing distribution shows that in the initial stages of the simulation there is a wide spread of cavity spacings. This is due to the fact that there are not as many cavities present initially as there are in the final stages of evolution and also that they are placed at random positions on the grain boundary thus giving a wide spread of spacings. However, as the system evolves the distribution of spacings become smaller. This is expected as the number of cavities has increased as well as the fact that
the cavities have grown and coalesced together. This means that there is less grain boundary remaining and that the spacings have become more uniform.

Cavity radii distribution

Cavity spacing distribution

25% Damage

40% Damage

75% Damage

Figure 88. Size and spacing distributions for stress = 50 MPa, \( \frac{M_s}{M_g} = 10, \ \psi = 120^\circ, \ \dot{N} = 4.569 \times 10^{-4} \ \text{s}^{-1}. \)
Figure 89. Cavity evolution for applied stress = 50 MPa, \( \frac{Ms}{Mgb}=10, \theta=120^\circ, N=4.569\times10^4 \text{ s}^{-1} \).

Figure 89 gives a representation of the cavities on the grain boundary at the three damage fractions previously defined. These plots were produced using a program written by the author that reads in a data file from the simplified finite element computer program and generates the system. In the figures, a dark band is used to represent each individual cavity. The length of the band is the cavity length and the height of the band is calculated to represent the height of the cavity at the midpoint. Figure 89 only shows 20% of the total grain boundary. This was due to the size of the cavities; if the whole grain boundary were plotted it would be very difficult to see the cavities in the initial stages of the system evolution. It can be seen from the figure that the system is not uniform, with multiple sizes and spacings of cavities. This confirms what is shown in Figure 88 and also that the
assumption of a uniformly arranged system of cavities is not a valid one. This is especially true in the initial stages of damage evolution.

Figure 90 shows the distribution of cavity radii on the left and the distribution of cavity spacing on the right for an applied stress of 5000 MPa. For the cavity radii distribution each bar represents a range of $2 \times 10^{-2}$ mm, and for the cavity spacing distribution each bar represents a range of $2 \times 10^{-3}$ mm. Despite the applied stress being unrealistic 5000 MPa
was used to push the model to an extreme, to investigate if the trends were the same. It can be seen from Figure 90 that the trends are the same as in the previous figure i.e. the distribution of cavity sizes increases with time and the distribution of cavity spacings decreases with time.

![Cavity evolution for applied stress = 5000 MPa, Ms/Mg=10, Ψ=120°, Ñ=4.569x10^-4 s^-1.](image)

Figure 91 shows the cavity evolution for an applied stress of 5000 MPa. Again, only 20% of the grain boundary is shown. It can be seen that under such an extreme applied stress the cavities become very 'crack-like' in shape very quickly. There is also a great deal of coalescence between cavities and hence the number of cavities present on the grain boundary is reduced. This results in larger cavities being formed and then propagating more quickly. It can also be seen that the system is not uniform in its evolution. Once
more, this shows that even under an extreme stress the system cannot be said to be uniform and to assume that it was would not be a valid assumption.

Finally, the contributions to the damage fraction from nucleation alone in the 'smeared-out' model are investigated for the cases discussed above. As stated in section 6.3 the graphs will not be presented in order to save space. Instead Table 6-1 shows the contributions to the total damage fraction from nucleation at the end of the simulation when the total damage had reached 80%.

<table>
<thead>
<tr>
<th>Applied Stress (MPa)</th>
<th>Contribution to total damage from nucleation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>34.1</td>
</tr>
<tr>
<td>50</td>
<td>23.4</td>
</tr>
<tr>
<td>500</td>
<td>24.3</td>
</tr>
<tr>
<td>5000</td>
<td>24.3</td>
</tr>
</tbody>
</table>

Table 6-1. Contributions to damage fraction from cavity nucleation.

It can be seen that the nucleation mechanism makes a major contribution to damage evolution. This is not true in reality. The percentage damage also remains approximately constant throughout the range of applied stresses. This basically explains the difference between the 'smeared-out' model and the simplified finite element model.

**Case 2** - $M_g = 2.08 \times 10^{-15}$, $M_{gb} = 2.08 \times 10^{-17}$, $M_g/M_{gb} = 100$.

The only difference between this case and the previous case is that the ratio of mobility $M_g/M_{gb}$ is increased from 10 to 100. All the other parameters are unchanged, that is, we take dihedral angle $= 120^\circ$ and nucleation rate $\dot{N}$ of $4.569 \times 10^{-4}$ s$^{-1}$. The values of applied stress used were 10, 50, 500 and 5000 MPa. This simulation was designed to investigate the effect of increasing the ratio of mobility on the comparison between the 'smeared-out' model and the simplified finite element model.

Figure 92 shows the damage evolution for both of the models at the different applied stresses. The results produced are very similar to those in case 1 with the 'smeared-out' model only agreeing with the simplified finite element model at the very high stress. It
can also be seen that the percentage differences are very similar to those in case 1, with two of the differences being larger, (47% compared to 34% and 55% compared to 43%). Therefore increasing the ratio of mobility does not seem to make any impact in terms of agreement between the two models.

Figure 92. Damage evolution for 'smeared-out' and simplified finite element models.

Figure 93. Separation velocity for 'smeared-out' and simplified finite element models.
Figure 93 shows the separation velocities for case 2. These confirm the conclusions drawn from the previous figure as well as the previous case. Table 6-2 shows the contributions to the total damage fraction from nucleation calculated for the 'smeared-out' model using Equation (6.2-11) at the end of the simulation when the total damage had reached 80%.

<table>
<thead>
<tr>
<th>Applied Stress (MPa)</th>
<th>Contribution to total damage From nucleation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>32.8</td>
</tr>
<tr>
<td>50</td>
<td>22.1</td>
</tr>
<tr>
<td>500</td>
<td>23.0</td>
</tr>
<tr>
<td>5000</td>
<td>23.0</td>
</tr>
</tbody>
</table>

It can be seen from Table 6-2 that the trend is the same as that in Table 6-1. There is the initial drop in contribution between the applied stress of 10 and 50 MPa after which the contribution remains approximately constant. The contribution values in this table are slightly less than those in the previous case. This is probably due to the higher value of $\frac{M_e}{M_{gb}}$ meaning that the cavities remain spherical for longer and thus the nucleated cavities are smaller.

6.4.3 Approaching the growth controlled limit by decreasing the nucleation rate.

**Case 3** - $M_s = 2.08 \times 10^{-16}$, $M_{gb} = 2.08 \times 10^{-17}$, $\frac{M_e}{M_{gb}} = 10$.

The third simulation used the parameters: $\frac{M_e}{M_{gb}} = 10$, dihedral angle = $120^\circ$ and an applied stress of 50 MPa. The nucleation rate was reduced from the $\dot{N} = 3.467 \times 10^{-3}$ s$^{-1}$ down to $2 \times 10^{-7} \dot{N}$. This simulation was designed to show the effect of nucleation rate on the damage evolution of the system. As the nucleation rate gets smaller and smaller it’s contribution to the damage process becomes smaller as far as the 'smeared-out' model is concerned and the two models should agree more closely.

Figure 94 shows the damage evolution for the simplified finite element and 'smeared-out' models for the 6 different nucleation rates used. As the nucleation rate is decreased
(moving from A to F on the graphs), the percentage difference in rupture time also decreases from a peak value of 45% down to 9%. This is consistent with the predictions of what should happen as the nucleation rate is being reduced, namely its' contribution to the damage evolution is also being reduced as there are less cavities being nucleated.

Figure 94. Damage evolution for 'smeared-out' and simplified finite element models.

Figure 95. Separation velocity for 'smeared-out' and simplified finite element models.
Figure 95 confirms the conclusions drawn from the previous figure and it can be seen that the separation velocities from the two models also become closer as the nucleation rate is reduced. It can also be seen that the maximum values of separation drop as the nucleation rate is decreased. This is due to there being less cavities present and hence there are less sources of material to allow the grains to separate. The characteristic diffusion length is also a determining factor. As the number of cavities increase so the diffusion length becomes shorter. The separation velocity is proportional to the inverse of the diffusion length cubed, therefore, as it decreases the separation velocity increases drastically.

Table 6-3 shows the contributions to the total damage fraction from nucleation at the end of the simulation when the total damage had reached 80%. The value of the contribution to damage from nucleation follows the same trends as identified in the previous cases. It tends to remain constant throughout the simulation despite the value of the nucleation rate being decreased.

<table>
<thead>
<tr>
<th>Fraction of nucleation rate (N_dot)</th>
<th>Contribution to total damage from nucleation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>23.4</td>
</tr>
<tr>
<td>$2 \times 10^{-3}$</td>
<td>23.8</td>
</tr>
<tr>
<td>$2 \times 10^{-4}$</td>
<td>23.9</td>
</tr>
<tr>
<td>$2 \times 10^{-5}$</td>
<td>23.6</td>
</tr>
<tr>
<td>$2 \times 10^{-6}$</td>
<td>22.7</td>
</tr>
<tr>
<td>$2 \times 10^{-7}$</td>
<td>20.4</td>
</tr>
</tbody>
</table>

There is a slight decrease in the contribution at the last value of nucleation rate, but by only 2%. This is despite the fact that there were only three cavities nucleated in the simplified finite element model and a similar number in the ‘smeared-out’ model. These results add weight to the conclusion that whatever the value of the nucleation rate in the ‘smeared-out’ model it will have a large contribution on the evolution of the system. As the nucleation rate was decreased the ‘smeared-out’ model began to agree more closely with the simplified finite element model. In this case the growth component of the smeared-out model was complimented by the nucleation component and gave a relatively close agreement with the simplified finite element model. However the nucleation rate
was set at a very unrealistic value that resulted in only three cavities being nucleated in the simplified finite element model.

**Case 4** - \( M_s = 2.08 \times 10^{-16}, M_{gb} = 2.08 \times 10^{-17}, M_s/M_{gb} = 100. \)

The final simulation used the parameters: \( M_s/M_{gb} = 100, \) dihedral angle = 120° and an applied stress of 20 MPa. Again, the nucleation rate was reduced from \( \dot{N} = 1.072 \times 10^{-3} \text{ s}^{-1} \) down to \( 2 \times 10^{-7} \dot{N}, \) (moving from A to F on the graphs). This simulation was investigating the effect of a lower applied stress and a higher mobility ratio on the damage evolution than the previous case.

![Figure 96](image)

**Figure 96.** Damage evolution for ‘smeared-out’ and simplified finite element models.

Figure 96 shows that as the mobility ratio is increased from 10 to 100 the percentage differences between the simplified finite element model and the ‘smeared-out’ increase across the whole range of nucleation rates used. This is in spite of reducing the applied stress from 50 MPa to 20 MPa. The increase in percentage difference between each simulation in case 4 and case 3 is approximately 13%. The best agreement achieved is 21% which is an acceptable difference in terms of life prediction but it is at an extremely unrealistic nucleation rate where there are no more than 5 cavities nucleated in the simplified finite element model.
Figure 97 shows the separation velocity for each simulation from both models. Again, it shows that the peak separation velocities reduce as the nucleation rate is reduced.

Finally, Table 6.4 shows the contributions to the total damage fraction from nucleation at the end of the simulation when the total damage had reached 80%. As in the previous case the value of the contribution remains approximately constant throughout at 22%. The trend is the same in that there is slight reduction in the final nucleation rate when there are very few cavities nucleated in the ‘smeared-out’ model.

Table 6-4. Contributions to damage fraction from cavity nucleation.

<table>
<thead>
<tr>
<th>Fraction of nucleation rate (N_dot)</th>
<th>Contribution to total damage from nucleation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>22.2</td>
</tr>
<tr>
<td>2E-3</td>
<td>22.1</td>
</tr>
<tr>
<td>2E-4</td>
<td>22.3</td>
</tr>
<tr>
<td>2E-5</td>
<td>22.1</td>
</tr>
<tr>
<td>2E-6</td>
<td>21.2</td>
</tr>
<tr>
<td>2E-7</td>
<td>18.7</td>
</tr>
</tbody>
</table>
6.4.4 2 Degree of freedom based ‘smeared-out’ model.

The use of the 1 degree of freedom model in the smeared out model was the first step in the analytical process. However, due to the model’s relative simplicity and low computational requirements it was thought that the accuracy could be improved by using the 2 degree of freedom model derived in chapter 4. This would allow more accurate modelling of the cavities as it allows the shape of the cavity to change from quasi-equilibrium to non-equilibrium or ‘nose’, depending on the applied conditions. The implementation was quite straightforward as the 2 degree of freedom model output values of $\dot{R}$ and $\dot{\Psi}$ which were used to determine the current values of $R$ and $\Psi$.

The results from the ‘improved smeared-out’ were not as expected. In the majority of cases there was no improvement at all between the rupture times of the two ‘smeared-out’ models and in some cases the improved model was worse than the original. The method used to compare the models was the evolution of damage fraction with time. The results from the simplified finite element model were graphed and used to calculate the percentage differences between the final rupture times for the ‘smeared-out’ models.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure98a.png}
\caption{Comparison of damage evolution from ‘smeared-out’ models for $\sigma = 10$ MPa, $M_s/M_{gb} = 1$, $\Psi = 120^\circ$.}
\end{figure}
Figure 98a shows the results from the 'improved smeared-out' model, original 'smeared-out' model and the simplified finite element model using data for copper shown in Appendix C, with: \( \sigma = 10 \text{ MPa} \), \( \Psi = 120^\circ \), \( M_s/M_{gb} = 1 \), \( L_T = 0.25 \text{ mm} \) and \( N = 4.57 \times 10^4 \text{ s}^{-1} \). It can be seen that there is a significant difference between the 'improved smeared-out' model and the original 'smeared-out' model. The 'improved smeared-out' significantly under predicts the lifetime and at the critical damage fraction of 80% the difference between the two 'smeared-out' models was 35%.

Figure 98b shows the comparison of damage evolution from 'smeared-out' models for \( \sigma = 10 \text{ MPa} \), \( M_s/M_{gb} = 1000 \), \( \Psi = 120^\circ \).

Figure 98b shows the comparison of 'smeared-out' models for the same system parameters as in Figure 98a with the exception of the ratio of mobilities, which has been increased to \( M_s/M_{gb} = 1000 \). It can be seen that there is no improvement achieved in the results with the 2 degree of freedom based smeared-out model even at the fast surface diffusion extreme.

Figure 98c shows the comparison of 'smeared-out' models for a higher applied stress of \( \sigma = 100 \text{ MPa} \) and other system parameters of: \( \Psi = 120^\circ \), \( M_s/M_{gb} = 1 \), \( L_T = 0.25 \text{ mm} \) and \( N = 1.01 \times 10^2 \text{ s}^{-1} \). Again it can be seen that the 2 degree of freedom model dramatically under-
estimates the rupture time compared with the 1 degree of freedom based model with a difference of 34% between the two.

Figure 98c. Comparison of damage evolution from ‘smeared-out’ models for \( \sigma = 100 \text{ MPa}, \frac{M_s}{M_{gb}} = 1, \Psi = 120^\circ \).

Figure 98d. Comparison of damage evolution from ‘smeared-out’ models, for \( \sigma = 100 \text{ MPa}, \frac{M_s}{M_{gb}} = 1000, \Psi = 120^\circ \).
Figure 98d shows the comparison of ‘smeared-out’ models for the same system parameters as in Figure 98c with the exception of the ratio of mobilities, which has been increased to $M_g/M_{gb} = 1000$. In this case it can be seen that the two ‘smeared-out’ models are in very close agreement with no improvement coming from the use of the 2 degree of freedom based ‘smeared-out’ model.

The reason for the decrease in accuracy was due to the way in which the ‘smeared-out’ model was derived. When the 2 degree of freedom based ‘smeared-out’ model was used it allowed the cavities to grow in a non-self similar manner, i.e. to develop a ‘nose’. This improves the accuracy of the growth component of the model but it also allows the nucleation component to nucleate large ‘crack-like’ cavities that grow rapidly and coalesce with the existing cavities. This has the effect of dramatically accelerating the damage evolution process and shortens the life of the system. It was for this reason that the 2 degree of freedom based ‘smeared-out’ model was not used in the comparison process, instead the original 1 degree of freedom based model was employed.
6.5 Conclusions.

The ‘smeared-out’ model has the advantage of requiring reduced computer processing power to complete a simulation compared with the simplified finite element model. Whereas the simplified finite element model can take hours to complete a simulation running on a mini-supercomputer the ‘smeared-out’ model only takes minutes running on a standard Pentium® III based PC. However, the ‘smeared-out’ model has a number of limitations. These were drawn from the comparisons and are as follows:

- For realistic values of applied stress and mobility the ‘smeared-out’ model significantly under-estimates the rupture life of material.
- Only when the applied stress is unrealistically high or the nucleation rate is unrealistically low does the ‘smeared-out’ model produce results that are in relatively good agreement with the simplified finite element model.
- The ‘smeared-out’ model exaggerates the contribution of cavity nucleation. The continuing increase in size of newly nucleated cavities causes the damage rate to accelerate sharply, thus under predicting the rupture life.
- The assumption of uniformly sized cavities and spacings has been shown to be unjustifiable in terms of damage evolution of the systems.
7. Effect of surface diffusion on creep damage.

7.1 Introduction.

Chuang et al., (1979), investigated the effect of surface diffusion on the evolution and rupture time of a pre-existing grain boundary cavity using a quasi-equilibrium model and comparing it to a ‘crack-like’ model. They concluded that the quasi-equilibrium mode of growth is favoured when the applied stress is low and the ratio of surface to grain boundary mobility ($M_s/M_{gb}$) is large. The ‘crack-like’ mode of growth is favoured when the applied stress is high and $M_s/M_{gb}$ is small. The effect of surface diffusion on the rupture time was also investigated and the conclusions drawn were that, as $M_s/M_{gb}$ was increased, the rupture time increased and approximately followed a $(M_s/M_{gb})^{3/2}$ law. This was true for the ‘crack-like’ and the quasi-equilibrium models. They also found that the rupture lifetime was reduced as the number of cavities was increased.

The effect of surface diffusion on multi-cavity growth and interaction has not been well documented. One of the main advantages of the simplified finite element model is that it includes contributions from both surface and grain boundary diffusion. This chapter investigates how the surface diffusion effects the overall rupture times for various applied stresses. The effect on damage evolution and separation velocity is also explored.

The rupture times are presented in the form of tables (as shown by Table 7-1 and Table 7-2). A separate table is used for each dihedral angle. The tables give rupture times in seconds for each value of applied stress $\sigma$, and ratio of mobility $M_s/M_{gb}$. For the purposes of producing the graphs showing the rupture times as a function of the mobility ratio, a normalised rupture time is used. This allows the effect of the mobility ratio to be shown clearly.
7.2 Rupture time predicted by the simplified finite element model.

This section has been split up into two subsections for a dihedral angle of 120° and 150° respectively. This allows the comparisons to be made more easily and the effect of differing dihedral angles to be investigated later in the section.

7.2.1 Parameters used in computer simulations.

The parameters that are used throughout the computer simulations require explanation before the results are presented. Unless otherwise stated the values listed here are used for all the simulations in this chapter. The first parameter is the timestep controlling value \( \alpha \), which is discussed in section 4.3.4. This value was determined empirically for these simulations and \( \alpha = 2 \times 10^6 \) was found to give the most acceptable results.

The total length of the system \( L_T \) was set as 0.25 mm. This is a relatively large grain size but the value is taken from Davanas and Solomon, (1990), who used data for copper in their simulations. This data is given in full in Appendix C and we adopt the same material parameters in this work. They are \( T = 1023K \), \( \gamma_s = 1.725 \times 10^3 \) J/mm\(^2\) with \( \gamma_{gb} = 1.725 \times 10^3 \) J/mm\(^2\) and \( \gamma_{gb} = 8.929 \times 10^{-4} \) J/mm\(^2\) for dihedral angles of 120° and 150° respectively.

The size of the cavity radius \( R \) was again based on the critical radius value with a scaling factor, \( \delta \), to ensure the cavities grew. The cavity radius is calculated using:

\[
R = \delta \frac{\gamma_s}{\sigma}
\]

There were three values of scaling factor \( \delta \), used in the simulations. This was due to the numerical instabilities that were encountered. For the stress of 10 MPa and below \( \delta = 1.3 \) was used, however, when the applied stress was increase to 20 MPa this was found to be insufficient with the faster surface diffusion cases. Therefore the value was increased to \( \delta = 2.3 \), which cured the problem. Finally for the stresses of 100 MPa and greater the value was increased to \( \delta = 10 \) to ensure that the newly nucleated cavities grew.
The remaining parameters that were used in the simulation and require explanation define the 'special lengths' that are defined in Appendix F. The first is the critical length for coalescence $l_{crit}$. This is defined as:

$$l_{crit} = 0.25 \left( \frac{\delta y_x}{\sigma} \right)$$

It can be seen that the critical length for coalescence is one quarter of the radius of a newly nucleated cavity. This value was determined empirically using a trial and error method. If it were changed it would have an impact on the rupture time.

The next parameter is the buffer zone length, $l_{buffer}$. This is used to form a 'buffer zone' around exiting cavities to prevent newly nucleated cavities being placed too close and coalescing instantly. The value chosen is also empirically derived and given by:

$$l_{buffer} = \left( \frac{\delta y_x}{\sigma} \right) \sin \frac{\Psi_{new}}{2}$$

where $\Psi_{new}$ is the dihedral angle of the newly nucleated cavities. It can be seen that the buffer zone length is equal to the half-length of a newly nucleated cavity. This prevents the 'clashing' of existing and newly nucleated cavities, which would cause problems in the computer program.

The final parameter to be defined here is the critical segment length $l_{seg}$, which determines the minimum length a section of grain boundary has to be to accept a newly nucleated cavity. If the section of grain boundary were too short, the nucleated cavity would 'clash' with existing ones and cause problems in the computer program. Once again this length is empirically derived and given by:

$$l_{seg} = 2 \left( \frac{\delta y_x}{\sigma} \right) \sin \frac{\Psi_{new}}{2} + 2l_{crit}$$

It can be seen that the critical segment length is given by the total cavity length of a newly nucleated cavity + twice the critical length. This allows a length of grain boundary either side of the new nucleated cavity to allow it to grow.
The nucleation rates used in these simulations are given in the results and were chosen so that they gave approximately 200 cavities during the lifetime of the system. This is a realistic number of cavities to have on a single grain boundary. All of the simulations began with a single pre-existing cavity placed at a random position on the grain boundary with a radius $R$, five times the critical value to ensure growth.

7.2.2 Rupture times for a dihedral angle of 120°.

The rupture time is defined by the time taken for the creep damage to reach 80%. Table 7-1 shows the rupture times for the 120° dihedral angle. The ratio of mobility and applied stress values are in the range of validity for this model as defined in chapter 4. The blank entries are where there were no simulations run for those parameters. This was mainly due to time constraints and the fact that at the extreme values of mobility ratio the simulations were very slow.

<table>
<thead>
<tr>
<th>Nucleation rate $\dot{N}$ (s⁻¹)</th>
<th>Applied stress (MPa)</th>
<th>$M_s$ (mm⁴/s/Kg)</th>
<th>$M_{gb}$ (mm⁴/s/Kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$4.57 \times 10^{-4}$</td>
<td>10</td>
<td>$2.08 \times 10^{-18}$</td>
<td>$2.08 \times 10^{-17}$</td>
</tr>
<tr>
<td>$1.07 \times 10^{-3}$</td>
<td>20</td>
<td>$2.08 \times 10^{-16}$</td>
<td>$2.08 \times 10^{-15}$</td>
</tr>
<tr>
<td>$2.18 \times 10^{-3}$</td>
<td>35</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$3.47 \times 10^{-3}$</td>
<td>50</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$6.48 \times 10^{-3}$</td>
<td>80</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$1.01 \times 10^{-2}$</td>
<td>100</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$2.49 \times 10^{-2}$</td>
<td>200</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$8.50 \times 10^{-2}$</td>
<td>500</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
<tr>
<td>$2.82 \times 10^{-1}$</td>
<td>1000</td>
<td>$2.08 \times 10^{-17}$</td>
<td>$2.08 \times 10^{-16}$</td>
</tr>
</tbody>
</table>

If one looks at the rows of the table the trend for the rupture times as a function of $M_s/M_{gb}$ is less clear. It can be seen that the rupture time is reducing for some the cases as well as increasing for others. A ‘common sense’ approach would expect that as the surface
mobility was increased a subsequent increase in the damage accumulation would occur. It
could be argued that the two diffusion processes, (surface and grain boundary diffusion)
are consecutive, i.e. each process has to occur in sequence before the system can change.
Therefore, accelerating one of the processes would in the very least not reduce the damage
growth. As can be seen from Table 7-1 this common sense argument has been found to be
incorrect.

During the validation of the 2 degree of freedom model in chapter 4, it was found that the
above argument is not necessarily correct. The model showed that as the surface mobility
was increased the rupture time was also increased. That is, increasing surface mobility
retarded the damage growth. The main reason for this is the ‘blunting’ effect that the
surface mobility has on the cavities present on the grain boundary.

![Figure 99. Cavity profile for \( \sigma = 500 \, \text{MPa}, M_s/M_{gb} = 1.0, \Psi = 120^\circ \) showing ‘crack-like’
growth from 2 degree of freedom model and full finite element model.]

At slow surface mobilities the cavities tend to ‘nose’ and evolve into thin ‘crack-like’
cavities. An example of this type of growth from the 2 degree of freedom model is shown
in Figure 99.

![Figure 100. Cavity profile for \( \sigma = 500 \, \text{MPa}, M_s/M_{gb} = 3000, \Psi = 120^\circ \) showing
‘blunted’ cavity growth for different cavity models]
However, as the surface mobility is increased the cavities are ‘blunted’, i.e. instead of the cavities evolving into ‘crack-like’ cavities they tend to grow in a ‘self-similar’ manner retaining their dihedral angles throughout the growth process. Figure 100 shows an example of the ‘blunted’ cavity growth from the 2 degree of freedom model.

This means the cavities are retaining their quasi-equilibrium shape. In this case a significantly larger amount of material has to be diffused along the free surface and into the grain boundary in order for the damage to be equivalent to that of a ‘crack-like’ cavity. This process takes a longer period of time and thus results in an increased time to failure.

Figure 101 by Chuang et al., (1973) shows the two types of growth that were discussed previously and confirms the results shown in Figure 99 and Figure 100. The cavity profile examples shown are for a single cavity simulation. However, the simplified finite element model predicts similar results.

Table 7-1 shows that the ‘common-sense’ argument is only true for the lower applied stresses. The 10 MPa and 20 MPa rows show that as the ratio of surface to grain boundary mobility \((M_g/M_{gb})\), is increased from 0.1 to 1, the rupture time decreases and then remains approximately constant as the ratio is increased further. Whereas for higher applied stresses \((>35\text{MPa})\), Table 7-1 shows that as the surface diffusion is accelerated the rupture time increases.

Figure 102 shows the relationship between the normalised rupture times and the ratio of surface to grain boundary mobility \((M_g/M_{gb})\) for the selected applied stresses. All the rupture times have been normalised by the rupture times for \(M_g/M_{gb}=0.1\) at the selected
stress level. Three cases have been selected to highlight the three different scenarios that have been observed from the results. The three scenarios are:

1. Rupture time increases dramatically with increasing $M_s/M_{gb}$.
2. Rupture time remains approximately constant with increasing $M_s/M_{gb}$.
3. Rupture time decreases with increasing $M_s/M_{gb}$.

![Graph showing normalized rupture times as a function of mobility ratio ($M_s/M_{gb}$) for a dihedral angle of 120°.](image)

**Figure 102. Normalised rupture times as a function of mobility ratio ($M_s/M_{gb}$) for a dihedral angle of 120°.**

The first case shown in Figure 102 is for an applied stress of 500 MPa. This is a relatively large applied stress and was used to test the model and determine whether or not the trend of increasing rupture time with $M_s/M_{gb}$ continued. It can be seen that the trend does indeed continue with a more pronounced increase in rupture time as the surface mobility is increased. Figure 102 shows that the rupture time has approximately increased by a factor of 1.8 from an initial value of $M_s/M_{gb} = 0.1$ to a final value of $M_s/M_{gb} = 100$.

Figure 103 shows the effect of $M_s/M_{gb}$ on the damage evolution for $\sigma = 500$ MPa. It can be seen that as the surface diffusion is accelerated the time taken to reach the critical damage fraction is also increased. As the ratio of $M_s/M_{gb}$ is continually increased the subsequent increase in final rupture time can be seen to be increasing at a larger rate. The graph also shows that at the beginning of the simulations there is very good agreement in the evolutions for all values of $M_s/M_{gb}$. This suggests that the effect of surface mobility is
at a maximum in the later stages of evolution, i.e. when there has been significant cavity growth and coalescence.

Figure 103. Damage evolution for applied stress = 500 MPa.

Figure 104 shows the effect of $M_s/M_{gb}$ on the separation velocity for the applied stress of 500 MPa, it can be seen that the same trend as discussed in the damage evolution exists...
again. An increasing $M_s/M_{gb}$ results in a decrease in separation velocity. This is consistent with a prolonged time to failure as the surface diffusion is being retarded and so takes longer to reach the same damage fraction. This is due to the fact that as the value of $M_s/M_{gb}$ is increased the cavities tend to stay more spherical during their growth. Figure 105 shows the evolution of dihedral angle with time for an applied stress of 500 MPa. It clearly shows the two types of growth discussed previously; the first is where the cavity remains spherical and so the dihedral angles remains constant, the second is the ‘crack-like’ growth where the dihedral angle decreases as the cavity becomes more ‘crack-like’ in shape.

![Figure 105. Dihedral angle evolution as a function of mobility ratio for $\sigma = 500$ MPa.](image)

This results in there being a larger number of spherical cavities present that occupy an equivalent amount of grain boundary to the ‘crack-like’ cavities. The final outcome of this is that there are a larger number of sources from which material can diffuse into the grain boundary. However, as the surface diffusion has been retarded it takes a longer amount of time for the material to reach the grain boundary and cause the grains to separate.

For a lower applied stress such as 100 MPa the trend is less pronounced. Figure 102 shows that the rupture time increases slightly as the surface mobility is increased and then remains approximately constant. Figure 106 shows the damage evolution for this case. It
can be seen that the effect of $M_s/M_{gb}$ on the damage growth is much less clear than in the previous case. Simulations D, E and F are almost identical in evolution with only a large increase in rupture time for the largest value of $M_s/M_{gb}$.

![Figure 106. Damage evolution for applied stress = 100 MPa.](image1)

![Figure 107. Separation velocity for applied stress = 100 MPa.](image2)
The results from Figure 106 show that the value of surface diffusion seems to have a less pronounced effect on the rupture time for a lower value of stress. Figure 107 shows the separation velocity for the same case. It can be seen that the same trend as described in Figure 104 exists except that the results are a lot closer together with the exception of the last simulation where $M_s/M_{gb} = 1 \times 10^6$.

The two cases that have been discussed have followed the trend discovered when validating the 2 degree of freedom model, i.e. increasing values of surface mobility lead to an increase in times to failure for most of the practical cases. However, the final case discussed for $\sigma = 10$ MPa follows the 'common sense' reasoning which is the reverse of the above trend. It can be seen in Figure 102 that when the applied stress is relatively low, ($\approx 10$ MPa), the rupture time decreases with increasing mobility ratio and then remains approximately constant.

Figure 108 shows the damage evolution for an applied stress of 10 MPa. What is immediately noticeable is the closeness of all of the rupture times.

![Figure 108. Damage evolution for applied stress = 10 MPa.](image)
This is a relatively low applied stress and as such the cavities tend to remain spherical even at the lower values of surface diffusion. The result of this is that there is very little ‘nosing’ of cavities and so the differences between the subsequent values of $M_g/M_{gb}$ are relatively small. Again it can be seen that the simulated results are all very close to each other during the first 40% of damage accumulation and it is only towards the end of the lifetime that there is a small deviation between simulations.

The main difference between this case and the previous two is the trend of the rupture time with increasing values of surface mobility. This trend is also visible in the separation velocities shown by Figure 109. There is a definite reversal or ‘switch’ in the way the rupture times vary with surface mobility. After the initial reduction in rupture time when the value of $M_g/M_{gb}$ is increased from 0.1 to 1 the results from the simulations remain very close together. This is also shown in Figure 109.

Figure 110 shows the evolution of dihedral angle for an applied stress of 10 MPa. It can be seen that for a low applied stress such as 10 MPa the cavities do in fact remain spherical throughout the lifetime of the simulation as the dihedral angle remains constant for both the fast and slow surface diffusion cases. This confirms the conclusions drawn
from the two previous figures and also gives a reason for the closeness of all the rupture
times. With the results given by Figure 110 it is now confirmed that there is very little
‘nosing’ of the cavities during the evolution. The absence of the ‘nosing’ effect explains
why there is no difference in acceleration of damage accumulation between the cases
presented in Figure 108.

Figure 110. Dihedral angle evolution as a function of mobility ratio for $\sigma =10$ MPa.
7.2.3 Rupture times for a dihedral angle of 150°.

Table 7.2 shows the rupture times for the 150° dihedral angle. As before the blank entries represent cases that were not run due to time constraints or the simulations themselves being too slow. As in the case for a 120° dihedral angle there are some selected cases presented to highlight the different trends found in the results of the simulations. The material and simulation parameters are the same as those used in the previous section.

<table>
<thead>
<tr>
<th>Nucleation rate $\dot{N}$ (s⁻¹)</th>
<th>$M_s$/Mgb</th>
<th>0.1</th>
<th>1</th>
<th>10</th>
<th>1×10⁷</th>
<th>1×10⁹</th>
<th>1×10¹¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>Applied stress (MPa) Rupture time (seconds)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.49×10⁻⁴</td>
<td>5</td>
<td>2.74E+07</td>
<td>2.76E+07</td>
<td>2.84E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.42×10⁻⁴</td>
<td>10</td>
<td>2.44E+06</td>
<td>2.44E+06</td>
<td>2.74E+06</td>
<td>2.74E+06</td>
<td>2.56E+06</td>
<td>2.58E+06</td>
</tr>
<tr>
<td>8.04×10⁻⁴</td>
<td>20</td>
<td>2.73E+05</td>
<td>2.57E+05</td>
<td>2.64E+05</td>
<td>2.64E+05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.64×10⁻³</td>
<td>35</td>
<td>1.48E+05</td>
<td>1.44E+05</td>
<td>1.54E+05</td>
<td>1.58E+05</td>
<td>1.88E+05</td>
<td></td>
</tr>
<tr>
<td>2.61×10⁻³</td>
<td>50</td>
<td>9.38E+04</td>
<td>9.36E+04</td>
<td>9.88E+04</td>
<td>1.01E+05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.58×10⁻³</td>
<td>100</td>
<td>3.25E+04</td>
<td>3.17E+04</td>
<td>3.45E+04</td>
<td>3.49E+04</td>
<td>3.39E+04</td>
<td>3.42E+04</td>
</tr>
<tr>
<td>1.87×10⁻²</td>
<td>200</td>
<td>1.18E+04</td>
<td>1.25E+04</td>
<td>1.38E+04</td>
<td>1.46E+04</td>
<td>1.55E+04</td>
<td></td>
</tr>
<tr>
<td>6.33×10⁻²</td>
<td>500</td>
<td>3.31E+03</td>
<td>3.77E+03</td>
<td>4.60E+03</td>
<td>5.93E+03</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Looking at Table 7-2 one can see that the rupture times are larger for the 150° dihedral angle than for the 120° dihedral angle. This is due to the fact that the cavity is more spherical than the previous case and so it is necessary to diffuse more material away from the free surface and onto the grain boundary for the equivalent amount of damage to occur. This takes longer to happen and so the rupture time is increased.

Now, if one looks at the rows of Table 7-2 the trend for the rupture time as a function of $M_s$/Mgb becomes more difficult to determine than the 120° results. Figure 111 shows the relationship between the normalised rupture times and the ratio of surface to grain boundary mobility. All the rupture times are normalised by rupture times for $M_s$/Mgb =0.1
at the selected stress level. In this section the applied stresses selected are 200, 100 and 10 MPa. These were selected because they gave the best demonstration of the trends.

**Figure 111.** Normalised rupture times as a function of mobility ratio ($M_s/M_{gb}$) for a dihedral angle of 150°.

**Figure 112.** Damage evolution for applied stress = 200 MPa.
The first case shown is for an applied stress of 200 MPa. This is the relatively high value of applied stress designed to push the model to the extreme. Figure 112 shows the effect of $M_s/M_{gb}$ on the damage evolution for this case. It can be seen from Figure 112 that the damage accumulation follows the same trend as in the 500 MPa case for the 120° dihedral angle. The times to failure all increase with increasing surface mobility. However, in this case the simulations are all quite similar in spacing for the final rupture times. There is no increase in rupture time by a larger amount as the surface mobility is increased. Figure 111 shows that the relationship between normalised rupture time and $M_s/M_{gb}$ is approximately linear although this may not be the case for further values of $M_s/M_{gb}$. Figure 113 shows the effect of $M_s/M_{gb}$ on the separation velocity for this case. It can be seen that it decreases as $M_s/M_{gb}$ increases.

Figure 113. Separation velocity for applied stress = 200 MPa.

Figure 114 shows the evolution of dihedral angle for an applied stress of 200 MPa. It can be seen that the cavities indeed remain spherical when the surface diffusion is fast, as the dihedral angle is remaining constant throughout the lifetime. It also shows that in the case of slow surface diffusion the cavities tend to evolve into thin ‘crack-like’ cavities as the dihedral angle can be seen to reduce as the creep damage accumulates.
The next case to be presented is for an applied stress of 100 MPa. Figure 111 shows that the relationship between normalised rupture time and $M_g/M_{gb}$ is not straightforward. The graph shows that the rupture time oscillates between increasing and decreasing values for an increase in $M_g/M_{gb}$. The reason for this is not known but it may be a computational problem on the part of the model. Newly nucleated cavities have been found to oscillate between growth and shrinkage before finally going one way or the other and this could be the outcome when compared with subsequent simulations.

Figure 115 shows the effect of $M_g/M_{gb}$ on the damage evolution for this case. It can be seen that there has been some 'switching' between the simulations and this highlights the oscillation discussed previously. It can be seen that the simulated results are very close in the initial stages of damage accumulation with a small deviation in the latter stages.

Figure 116 shows the effect of $M_g/M_{gb}$ on the separation velocity for an applied stress of 100 MPa. The results are very close together for all cases and the main question that arises from the graph is why the separation velocities are similar for the four largest values of $M_g/M_{gb}$. In these cases the peak number of cavities was very similar at approximately
215, whereas in the other two cases it was much lower at approximately 190 and 180. This accounted for the differences in separation velocity.

Figure 115. Damage evolution for applied stress = 100 MPa.

Figure 116. Separation velocity for applied stress = 100 MPa.
The final case discussed is for an applied stress of 10 MPa. Figure 111 shows that the rupture time does not follow a simple trend as $M_s/M_{gb}$ is increased. It can be seen to remain approximately constant when $M_s/M_{gb}$ is increased from 0.1 to 1 after which it increases when $M_s/M_{gb}=10$, only to decrease again as $M_s/M_{gb}$ is further increased. After the results from the low applied stress for the 120° case it cannot be ruled out that there is a computational problem involved or that at low applied stress there is not an observable trend.

![Diagram showing damage evolution for applied stress = 10 MPa.](image)

**Figure 117. Damage evolution for applied stress = 10 MPa.**

Figure 117 shows the effect of $M_s/M_{gb}$ on the damage evolution for the above case. It can be seen that as in previous cases there is very good agreement between the simulated results in the initial stages of the damage evolution. The divergence starts to occur at approximately 20%. There is not a definite pattern in the way the rupture times vary with increasing $M_s/M_{gb}$, although it can be said that the rupture time does decrease from the peak value and continues to decrease as $M_s/M_{gb}$ gets larger. The same conclusions can be drawn from Figure 118, which shows the effect of $M_s/M_{gb}$ on the separation velocity for this case.
Chapter 7 Effect of Surface Diffusion on Creep Damage.

Figure 118. Separation velocity for applied stress = 10 MPa.

![Graph showing separation velocity for various mobility ratios.]

Figure 119. Dihedral angle evolution as a function of mobility ratio for $\sigma = 10$ MPa.

![Graph showing dihedral angle evolution.]

The final figure presented shows the evolution of dihedral angle for an applied stress of 10 MPa. Figure 119 shows that the trend is very similar to the $120^\circ$ case given by Figure 110, i.e. the cavities tend to remain spherical for the majority of the lifetime for low
applied stresses. This confirms the assumption that the cavities do remain spherical at low applied stress irrespective of the value of the dihedral angle.
7.3 Conclusions.

The effect of surface diffusion on creep damage has been investigated in this chapter and the results presented have shown that the surface diffusion does indeed have a significant effect on the rupture time, although it is not a straightforward relationship.

The surface diffusion has been shown to have two opposing effects on the rupture times depending on the applied level of stress. In the majority of cases it was shown to increase the rupture times as the value of surface diffusion was increased. The actual increase was shown to vary with the applied stress value; as the applied stress was increased the effect of surface diffusion was increased. The increases in rupture time range from 20% to 184% depending on the applied level of stress. The higher the applied stress, the higher the increase was found to be. In the case of the lower applied stresses (≤ 20 MPa), it was shown that increasing $M_s/M_g$ decreases the rupture time, although only by a maximum of 8.5%.

The results for the 120° dihedral angle were relatively easy to draw conclusions from as the trends were easily identified from the data. The results from the 150° dihedral were more erratic. The higher applied stresses followed the same trends as those from 120° but there was a wide variation in the rupture time for the lower applied stress values, with the results oscillating from increasing to decreasing times to failure. The value of 150° is not a particularly realistic one as the cavities are usually more penny-shaped and the value of 120° is more appropriate for most of the materials.

From the numerical results shown in this chapter, it can be concluded that one should select or design a material which possesses fast surface diffusivity in order to obtain a high resistance to diffusional damage growth. This is a surprising conclusion but it is consistent with the numerical findings in this chapter. For the majority of the cases, increasing the surface diffusivity leads to more equilibrium (rounded) shaped cavities as opposed to the ‘crack-like’ cavities. It is more difficult for the equilibrium shaped cavity to grow (more material has to be re-distributed by solid state diffusion). This effect
overcomes the effect of a faster movement of material along the cavity surface and prolongs the time to failure.

Chuang et al., (1979) looked at the cases of fast and slow surface diffusion as well as producing a model which simulated the intermediate case between the two extremes and obtained a semi-analytical model solution by linearising the governing equations. This semi-analytical model is very instructive in judging which of the extreme models work under a particular combination of applied stress and relative diffusivity. The models by Chuang et al., (1979) are however, only for single cavity systems and, as a result do not take into account the interactions of cavities when they become very close to one another and coalesce. Also, due to the complexity of these models it would be very difficult to extend them to be able to simulate multi-cavity systems.

The results presented in this chapter tend to agree with the general observations made by Chuang et al., (1979), in that with the increasing ratio of surface to grain boundary diffusion comes an increase in rupture time. The results from the single cavity 2 degree of freedom model, as well as the multi-cavity model also showed that the shape of cavity evolution varies with applied stress levels. It has been shown that at high applied stresses the cavities evolve to ‘crack-like’ shapes, and at low applied stresses they tend to remain spherical, this was found to be the case by Chuang et al., (1979). At the intermediate applied stress levels it has been shown that the cavities tend to remain spherical shaped until the final stages when there is some reduction in dihedral angle and the cavity becomes slightly ‘crack-like’. The ‘switching’ effect which was discussed concerning the reduction of rupture times at the lower applied stresses was something that was not discussed by Chuang et al., (1979). This was only found to be present in the simplified finite element model with significant numbers of cavities and only at applied stresses less than 35 MPa. This indicates that it could be, in part, due to the interactions between the cavities as they coalesced and continued to evolve, something that the Chuang et al. model could not simulate being only for a single cavity.
8. Large ‘crack-like’ cavity evolution.

8.1 Introduction.

Recently Cocks and his co-workers (Cocks and Pan (1993), Pan and Cocks (1993), Cocks, Gill and Pan (1999), have evaluated the process of crack growth in a Coble creep material. In their work the propagation of a crack through an array of triple-point cavities lying directly ahead of the crack tip was simulated using a numerical technique.
Figure 120. (a) A microscopic crack in a polycrystalline material with deforms by Coble creep. (b), (c), (d) The geometry after increasing amounts of crack growth. Pan and Cocks, (2000).

Figure 120 shows the type of system used in the work. The boundaries shown in the figure are axes of symmetry. The four different views of the system represent the increasing amounts of crack growth. There are two mechanisms that contribute to the crack growth: the diffusion of material away from the crack and the growth of triple point cavities. The contribution from cavity growth results in the instantaneous increments of crack growth as the cavities coalesce with the crack.
Figure 121 shows the variation of crack length with time for the case shown in Figure 120. The vertical axis represents the crack tip position and steps in this curve indicate where a triple point cavity coalesced with the crack.

The results basically indicated that the creep life of the system is not determined by the presence of the dominant crack. There was no cavity nucleation in this model and only the triple point cavities were considered. The presence of the triple point cavities determined the lifetime of the system as they grew almost independently of the crack. The cavities nearest the crack tended to grow the fastest, however the cavities which were further away from the crack tip tended to ‘catch up’ towards the end of the lifetime and end with approximately the same growth rate. This resulted in the cavities being approximately all the same size at the time of final failure. This can be seen in Figure 120d, where there is a large amount of crack growth and the cavities ahead of the crack are clearly visible and similar.

![Figure 121. The variation of crack length and remote strain with time for the problem of Figure 120. Pan and Cocks, (2000).](image)

Figure 122 shows the detailed stress distribution along the line of grain boundary directly ahead of the crack tip for the case where no cavities were placed in the system for an applied stress of $\sigma = \sigma_0$ and zero capillarity stress at the crack tip. It can be seen from Figure 122 that the stress normal to the boundary increases sharply from zero at the crack
tip to $8.5\sigma_0$ over half the length of the first facet. It can also be seen that the peak and mean stresses undulate in magnitude with increasing distance ahead of the crack tip. Despite the high stress concentration in the vicinity of the crack-tip, the model predicts that the material fails by the simultaneous growth of the cavities instead of the propagation of the crack through the entire material.

![Stress vs Distance](image)

**Figure 122.** The variation of local stress with distance away from crack tip for the problem of Figure 120. Pan and Cocks, (2000).

The newly developed simplified finite element model is able to simulate a wide variety of cavity growth situations. Cavities of differing sizes and shapes are placed on the grain boundary prior to the simulation being run.

In this chapter, the simplified finite element model is used to investigate the interactions between a large ‘crack-like’ cavity and much smaller cavities on a single grain boundary. In the simulation a large ‘crack-like’ cavity, i.e. a crack, whose profile is long and thin is placed on the grain boundary with several small quasi-equilibrium cavities placed on either side of the ‘crack-like’ cavity. A remote stress is applied to the system. An example of the type of system used is shown in Figure 123.
The size and position of cavities, position and magnitude of applied stress and material parameters were all varied over a range of values to investigate the effect they had on the growth of the cavities, in particular the growth of the large 'crack-like' cavity.

The purpose here is to investigate the interaction between a large 'crack-like' cavity with the small cavities along a single grain boundary. Our particular interest is to investigate if the dominant crack propagates, if the grain boundary fails by the propagation of the large 'crack-like' cavity through the smaller ones or by the approximate simultaneous growth of the large and small cavities.

Figure 123. Example of a large 'crack-like' cavity system.
8.2 Local stress variation.

In order to investigate the growth of the cavities on the grain boundary, the local stress variation was calculated using the method derived in chapter 5.5. This shows how the local stress varies with position along the grain boundary. For a crack to propagate in a poly-crystal material there is normally a stress concentration directly ahead of the crack-tip. In this region the local stress is many times that of the applied stress, and it is this that causes the cavities ahead of the crack-tip to grow very rapidly and link-up with the crack. Figure 124 shows the local stress variation for a large 'crack-like' cavity.

![Figure 124. Local stress distribution for large 'crack-like' cavity for applied stress 20 MPa](image)

In this case the system consisted of one large 'crack-like' cavity with an applied stress of 20 MPa. The material parameters used are for copper and are given in Appendix C. The total length of the system is 0.25 mm with the centre of the cavity at 0.125 mm, with $M_s = 2.08 \times 10^{-15} \text{ mm}^4 \text{s kg}^{-1}$, $M_{gb} = 2.08 \times 10^{-17} \text{ mm}^4 \text{s kg}^{-1}$ giving the ratio of $M_s/M_{gb} = 100$. The 'crack-like' cavity has a radius, $R$, of 0.1 mm, a dihedral angle, $\Psi$, of 50°, $\gamma_s = 1.725 \times 10^{-3} \text{ J mm}^{-2}$ and $\gamma_{gb} = 3.127 \times 10^{-3} \text{ J mm}^{-2}$. It can be seen from the graph that the local stress is higher than the applied stress at the ends of the system, however, nearer to the cavity tip.
the local stress drops sharply until it is equal to the capillarity stress at the tip. There is not a significant stress concentration ahead of the large cavity on a single grain boundary. Figure 125 shows the local stress distribution for the case where six quasi-equilibrium cavities of approximately ten times the critical size for nucleation are placed on the grain boundary. This simulation uses the same material parameters as the previous case except for an applied stress of 40 MPa and $\gamma_{gb} = 8.929 \times 10^{-4}$ J mm$^{-2}$. The ratio of $M_f/M_{gb}$ is again 100, the dihedral angles were all 150° with the cavity radii $R = 1.1 \times 10^{-4}$ mm.

![Figure 125](image)

**Figure 125.** Local stress distribution for six quasi-equilibrium cavities for applied stress of 40 MPa.

It can be seen from Figure 125 that the local stress is parabolic in nature and reaches a maximum value midway between the cavities.

The reason for the lack of any stress concentrations ahead of the cavity tip is due to the fact that the stress distribution produced by the solid state diffusion model is the ‘steady-state’ solution. In this solution the instantaneous elastic stress concentration has been completely released by matter re-distribution along the grain boundary.
8.3 Interaction between the large and small cavities.

This section discusses the results obtained from the simplified finite element model for a variety of different scenarios concerning the interaction between a large ‘crack-like’ cavity and other small cavities.

The material parameters used in this section are for copper. Appendix C gives full details of the material data. The temperature is assumed to be 1024 K as used by Davanas and Solomon, (1990). This leads to the following values: $M_{gb} = 2.08 \times 10^{-17}$ mm$^4$ s kg$^{-1}$, $\gamma_s = 1.725 \times 10^{-3}$ J mm$^{-2}$, $\gamma_{gb} = 3.127 \times 10^{-3}$ J mm$^{-2}$ for a dihedral angle, $\Psi$, of 50°, and $\gamma_{gb} = 8.929 \times 10^{-4}$ J mm$^{-2}$ for a dihedral angle, $\Psi$, of 150°. The surface mobility, $M_{s}$, is varied from $M_{s} = 2.08 \times 10^{-17}$ to $M_{s} = 2.08 \times 10^{-15}$ mm$^4$ s kg$^{-1}$ depending on the required ratio of $M_s/M_{gb}$.

The system parameters used in these simulations are common to all of cases. The total length of the grain boundary, $L_{gb}$, is 0.25 mm. The dihedral angle of the large ‘crack-like’ cavity is 50° and for the smaller cavities it is 150°. The critical radius, $R_{crit}$, and the critical length for coalescence, $l_{crit}$, are calculated as in the previous chapter. That is, $R_{crit} = 5\gamma_s/\sigma$ and $l_{crit} = 0.25 R_{crit}$. The nucleation rate was chosen to give approximately 100 cavities over the lifetime of the system, this is a reduced number to take into account the presence of the large ‘crack-like’ cavity that is pre-existent on the grain boundary. The individual nucleation rates will be given for each case.

The first set of results is for a symmetrical system without cavity nucleation, i.e. the large cavity is placed in the centre of the grain boundary and the stress is also applied along the symmetric line of the grain. There are a number of equally sized, pre-existing cavities placed on either side of the ‘crack-like’ cavity to encourage propagation. Two values of applied stress, $\sigma$, are used: 20 MPa and 200 MPa. At each of the stresses the ratio of mobilities $M_s/M_{gb}$ is varied from 1 to 100 to investigate their effect on the damage evolution. Because of symmetry only the damage evolution for half of the grain boundary is presented.
CHAPTER 8 LARGE ‘CRACK-LIKE’ CAVITY EVOLUTION.

The second set of results is for a symmetrical system with cavity nucleation. This system does not have the pre-existing cavities present on the grain boundary. Instead, the cavities are nucleated continuously at random positions on the grain boundary. The same material parameters and applied stresses are used as in the previous cases. Again, only half of the system is shown.

The third set of results is for a non-symmetrical system with cavity nucleation. In this case the large ‘crack-like cavity is placed towards the right-hand side of the system with its centre at 0.18 mm from the left side instead of 0.125 mm as in the previous symmetric cases. The load is applied at a position of 0.06 from the left side making it off-centred. This has the effect of causing the system to try and open up more on the left side and close down or ‘pinch’ on the right. In this case the cavities should shift towards the opening side of the system and there should be very little cavity growth on the right side of the large ‘crack-like’ cavity. This type of system should also be most suited to crack propagation. The same applied stresses, $\sigma$, of 20 and 200 MPa are used, as well as the same values of $M_g/M_g$ of 1 and 100. The entire system is shown for these results as it is no longer a symmetrical system.

The results are presented in the form of plots from the program written by the author to display the data produced by the simplified finite element computer model. The plots show the cavities as rectangular blocks on the grain boundary as to plot each of them as truncated arcs would require more computer processing power. Each block represents a cavity in terms of its maximum dimensions in the vertical and horizontal directions.
8.3.1 Symmetrical system with pre-existing cavities and no nucleation.

**Case 1: \( \sigma = 20 \) MPa, \( M_g = 2.08 \times 10^{-17} \), \( M_{gb} = 2.08 \times 10^{-17} \), \( M_g/M_{gb} = 1 \).**

Figure 126 shows the evolution of the system for an applied stress of 20 MPa and a ratio of \( M_g/M_{gb} = 1 \). The pre-existing small cavities have radii, \( R = 4.46 \times 10^{-4} \) mm and dihedral angle, \( \Psi = 150^\circ \), and have a centre-to-centre spacing of \( 3.45 \times 10^{-3} \) mm. They can be clearly seen at the initial damage fraction of 44%. The large 'crack-like' cavity has a radius, \( R = 0.1 \) mm and dihedral angle, \( \Psi = 50^\circ \). The value of \( l_{cm} \) is \( 2.16 \times 10^{-5} \) mm. As the system evolves the smaller cavities grow rapidly, with the furthest from the 'crack-like' cavity tending to grow at the fastest rate.

![Figure 126. Cavity evolution for applied stress of 20 MPa and \( M_g/M_{gb} = 1 \).](image)

These cavities eventually coalesce to form a smaller 'crack-like' cavity. The cavity nearest the 'crack-like' cavity can be seen to grow at a slower rate than the others. This is
due to its proximity to the large 'crack-like' cavity, which is attempting to 'swallow' it. The peak number of cavities in this simulation was 31 and at the final damage fraction this had reduced to 29. The coalescence can be seen in the new 'crack-like' cavity on the left on the grain boundary that has grown the most. There can be seen to be very little growth in the 'crack like' cavity and at the final damage fraction it has only grown in length by 2.2%.

**Case 2: \( \sigma = 20 \text{ MPa}, M_g = 2.08 \times 10^{-15}, M_{gb} = 2.08 \times 10^{-17}, \frac{M_g}{M_{gb}} = 100. \)**

Figure 127 shows the evolution of the system for an applied stress of 20 MPa but with a ratio of \( \frac{M_g}{M_{gb}} = 100 \). The remaining system parameters used in this simulation are the same as those used in the previous case.

![Cavity evolution for applied stress of 20 MPa and \( \frac{M_g}{M_{gb}} = 100 \).](image)

Figure 127. Cavity evolution for applied stress of 20 MPa and \( \frac{M_g}{M_{gb}} = 100 \).
The same trend can be seen as in the previous case in that the small pre-existing cavities grow at the fastest rate, with the most distant ones from the 'crack-like' cavity coalescing to form mini-cracks. In this case there is a slight difference in the shape of the pre-existing cavities; due to the faster surface diffusion they tended to stay more spherical. This makes them appear less thin and accounts for their apparent increase in size.

In this simulation the peak number of cavities was 31 and, at the final damage fraction this had reduced to 15. If one compares the 44% and 60% damage fraction plots, it can be seen that the cavity nearest the crack 'disappears'. This cavity did not coalesce with the large 'crack-like' cavity; instead it 'healed' itself. In effect the large 'crack-like' cavity prevented it from growing and caused it to shrink until it was completely removed.

The 'crack-like' cavity grew by a larger amount than in the previous case. At the final critical damage fraction it had increased in length by 6.7%. This was purely growth as it can be seen from the results that there were no cavities 'consumed' by it. The smaller cavities in this simulation coalesced with each other instead of coalescing with the large 'crack-like' cavity.

**Case 3: \( \sigma = 200 \text{ MPa}, M_{gb} = 2.08 \times 10^{-17}, M_{gb} = 2.08 \times 10^{-17}, M_{gb}/M_{gb} = 1 \),**

Figure 128 shows the evolution for an applied stress of 200 MPa and a ratio of \( M_{gb}/M_{gb} = 1 \). This case uses a relatively large applied stress, which was chosen to push the model to the extreme. This case uses the same material and simulation parameters as those used in the previous case with the exception of the small cavity radii which was reduced to \( R = 2.23 \times 10^{-4} \text{ mm} \) and the centre-to-centre spacing, which was reduced to \( R = 8.63 \times 10^{-4} \text{ mm} \) to encourage to crack to propagate. The value of \( l_{cr} \) is also reduced to \( 2.16 \times 10^{-6} \text{ mm} \).

It can be seen from Figure 128 that the pre-existing cavities quickly coalesce to form a new long thin 'crack', which is then consumed by the existing 'crack-like' cavity to form a very large crack. It can be seen that the new large crack grows very quickly and at the critical damage fraction it has extended in length by 237% from its original length.
Due to the large applied stress it can be seen that there is a significant amount of cavity coalescence, between the smaller cavities as well as the large 'craclike' cavity. In this simulation the peak number of cavities was 31 and at the critical damage fraction this had reduced to 1, i.e. the large 'crack-like cavity had coalesced with all of the smaller cavities to form one very large 'crack-like' cavity.

\[ t = \frac{0}{40\% \text{ damage}} \]
\[ t = 6.04 \times 10^7 \text{s, } 60\% \text{ damage} \]
\[ t = 1.37 \times 10^8 \text{s, } 70\% \text{ damage} \]
\[ t = 2.72 \times 10^8 \text{s, } 80\% \text{ damage} \]

**Figure 128.** Cavity evolution for applied stress of 200 MPa and \( M_s/M_{gb}=1 \).

**Case 4: \( \sigma = 200 \text{ MPa, } M_s = 2.08 \times 10^{-15}, M_{gb} = 2.08 \times 10^{-17}, M_s/M_{gb}=100 \).**

Figure 129 shows the evolution of the system for an applied stress of 200 MPa and a ratio of \( M_s/M_{gb} =100 \). This case uses the same simulation and material parameters as those
used in the previous case. In this case, as before, the pre-existing cavities coalesce quickly to form another ‘crack-like’ cavity, which proceeds to grow rapidly. Due to the faster surface diffusion the cavities stay more spherical and so appear ‘thicker’ on the grain boundary.

\[
t = 0, \quad 40\% \text{ damage}
\]

\[
t = 3.09 \times 10^8 \text{s, } 60\% \text{ damage}
\]

\[
t = 3.8 \times 10^8 \text{s, } 70\% \text{ damage}
\]

\[
t = 4.44 \times 10^8 \text{s, } 80\% \text{ damage}
\]

Figure 129. Cavity evolution for applied stress of 200 MPa and \(M_d/M_{gb} = 100\).

These smaller cracks eventually coalesce with the large ‘crack-like’ cavity and form a larger crack, which continues to grow rapidly. It can be seen that the ‘crack-like’ cavity is much thicker than in the previous case. This shows that for the fast surface diffusion case the dihedral angle maintains a larger value. At the final damage fraction the ‘crack-like’ cavity had extended in length by 235%.

The peak number of cavities in this case was 31 and at the final critical damage fraction, this had reduced to 1. As in the previous case, only the large ‘crack-like’ cavity remained.
8.3.2 Symmetrical system with cavity nucleation.

Case 5: $\sigma = 20$ MPa, $M_s = 2.08 \times 10^{-17}$, $M_{gb} = 2.08 \times 10^{-17}$, $M_s/M_{gb}=1$.

Figure 130 shows the evolution for an applied stress of 20 MPa and a ratio of $M_s/M_{gb} = 1$. The main system and material parameters as well as the large ‘crack-like’ cavity are unchanged from the previous cases. The newly nucleated cavities have $R = 8.63 \times 10^{-4}$ mm and $\Psi = 150^\circ$. The value of $l_{cm}$ is $2.16 \times 10^{-4}$ mm. In this case there is also continuous random cavity nucleation throughout the lifetime of the simulation. The nucleation rate was chosen so that it gave approximately 50 cavities during the lifetime of the system. This was reduced to take account of the existence of the large ‘crack-like’ cavity and initial damage fraction of 34%.

If the nucleation rate was too large the damage evolution would be nucleation controlled and there would be very little diffusive growth. The nucleation rate chosen was
Chapter 8 Large 'crack-like' cavity evolution.

\( \dot{N} = 8.04 \times 10^{-6} \text{ s}^{-1} \). It can be seen that the nucleated cavities are smaller than the pre-existing cavities in the previous cases and there is not a large amount of growth.

The cavities are present on the grain boundary but they are too small to show up. This is the reason the 90% damage fraction does not appear to be 90% damaged. If one were to zoom in on the grain boundary the cavities would be visible. The cavities that are visible can be seen to coalesce with each other and form larger cavities. In this case due to the fact that the nucleation of cavities is random, the damage is localised on areas of the grain boundary.

At the final damage fraction the large 'crack-like' cavity had extended in length by 3.1%. The peak number of cavities on the grain boundary was 55 and at the critical damage fraction this had reduced to 48 through coalescence. This confirms the results of Pan and Cocks, (2000), in that the damage accumulation comes from the growth of the cavities as opposed to the propagation of the crack.

**Case 6:** \( \sigma = 20 \text{ MPa}, M_s = 2.08 \times 10^{-15}, M_{gb} = 2.08 \times 10^{-17}, M_s/M_{gb} = 100 \).

Figure 131 shows the evolution for an applied stress of 20 MPa and a ratio of \( M_s/M_{gb} = 100 \). The system and material parameters used in this case as well as the nucleation rate, \( \dot{N} \), are the same as those used in the previous case. In this case the nucleated cavities can be seen more easily than in case 5. This is due to the faster surface diffusion allowing the cavities to maintain a larger dihedral angle.

There is a significant amount of coalescence towards the later stages of the simulation, however there is no coalescence with the large 'crack-like' cavity. When the system reached the critical damage fraction the crack-like cavity had extended in length by 3%, which is very similar to the previous case.

In this case the peak number of cavities present on the grain boundary was 44 and at the critical damage fraction this had reduced to 36. This is a similar amount of coalescence to the previous case however, the extra 'thickness' of the cavities due to the faster surface diffusion in this case allow more of the coalesced cavities to be seen.
The nucleation rate was checked to ensure that it was not too fast so that the problem became nucleation controlled. The total length of all of the newly nucleated cavities was calculated, as well as the length of the large ‘crack-like’ cavity. This length was compared with the total length of the grain boundary and a 35% difference was found.

**Case 7: \( \sigma = 200 \text{ MPa}, M_g = 2.08 \times 10^{-17}, M_{gb} = 2.08 \times 10^{-17}, M_g/M_{gb} = 1 \).**

Figure 132 shows the evolution for an applied stress of 200 MPa and a ratio of \( M_g/M_{gb} = 1 \). Again, the main system and material parameters used in this case were the same as those used in the previous cases. The newly nucleated cavities had radii \( R = 8.63 \times 10^{-5} \text{ mm} \) and dihedral angle, \( \Psi^V = 150^\circ \). The value of \( l_{crit} \) is \( 2.16 \times 10^{-5} \text{ mm} \). The nucleation rate \( \dot{N} \) was again chosen to give approximately 50 cavities during the lifetime of the system. The value chosen was \( \dot{N} = 1.87 \times 10^{-4} \text{ s}^{-1} \). As in the previous cases this value was checked to ensure that the system was not nucleation controlled, and, as before it was found that there was a significant amount of growth in the newly nucleated cavities before failure.
The newly nucleated cavities are difficult to see on the grain boundary due to their small size. In this case, due to the large applied stress and slow surface diffusion they are being nucleated and remaining ‘crack-like’ in shape throughout their evolution.

These results are in stark contrast to those in case 3, where there was a large amount of growth and coalescence. The main reason for this is the size of the cavities. In case 3 they were pre-existing and quite large, whereas in this case they are being randomly nucleated at just above the critical radius value. At the final damage fraction the large ‘crack-like’ cavity had extended in length by 1.1%.

The peak number of cavities present on the grain boundary was 54 and at the critical damage fraction this number had reduced to 47. This is a very similar number of cavities and coalescence to case 5.
Case 8: \( \sigma = 200 \text{ MPa, } M_s = 2.08 \times 10^{-16}, M_{gb} = 2.08 \times 10^{-17}, M_s/M_{gb} = 100. \)

Figure 133 shows the evolution for an applied stress of 200 MPa and a ratio of \( M_s/M_{gb} = 100. \) This case uses the same material and simulation parameters and nucleation rate as the previous case.

![Diagram of cavity evolution](image)

Figure 133. Cavity evolution for applied stress of 200 MPa and \( M_s/M_{gb} = 100. \)

There is a clearly visible difference between the cavities in this case and those in case 7; in this case the nucleated cavities appear larger on the grain boundary and there is a significant amount of coalescence occurring in the later stages of damage accumulation. This has been the case for all the simulations with fast surface diffusion. This could be due to the presence of the more rounded cavities as opposed to the 'crack-like' cavities. It has been shown that in the fast surface diffusion cases the cavities grow by a larger amount. This would allow them to become larger and reach the neighbouring cavity and coalesce with it.

It can be seen in this case that the large 'crack-like' cavity has coalesced with some of the
smaller cavities as it has become 'thicker', this indicates that the dihedral angle has increased in order to maintain the same amount of damage after coalescence. At the critical damage fraction the larger 'crack-like' cavity had extended in length by 3% which is a similar amount to the previous cases. The peak number of cavities present on the grain boundary was 81 and at the critical damage fraction this had reduced to 63.

8.3.3 Off-centre loading with nucleation.

In the following cases the large 'crack-like' cavity is placed off-centre and the load is no longer applied at the midpoint but towards the left-hand edge of the system (Figure 134). The equivalent average stress is found by dividing the applied load by the total grain boundary length.

In this set of simulations the grains are permitted to rotate as well as separate. This has the result of 'squeezing' one end of the grain boundary and 'opening-up' the other. It is now necessary to plot the entire system (rather than half), and as a result of the larger scale the smaller cavities do not show up. This is why the majority of the damage can only be seen at the 80 and 90% damage fractions.

Figure 134. Example of off-centre cavity system.

The main material and system parameters are the same as those in the previous cases. The large 'crack-like' cavities radius has been reduced from $R = 0.1$ to $R = 0.08$ mm to allow more growth during the evolution. The dihedral angle is unchanged with $\Psi = 50^\circ$. The nucleation rates were chosen to give approximately 100 cavities on the grain boundary.
during the lifetime of the system. This is an increase on the previous cases due to the decrease in the size of the large 'crack-like' cavity. Individual nucleation rates are given for each of the cases. The dihedral angle for nucleated cavities has been reduced to 120°.

**Case 9:** $\sigma_{2y} = 20$ MPa, $M_a = 2.08 \times 10^{-17}$, $M_{gb} = 2.08 \times 10^{-17}$, $M_a/M_{gb} = 1$.

Figure 135 shows the evolution for an averaged applied stress of 20 MPa and a ratio of $M_a/M_{gb} = 1$. The main material and simulation parameters are the same as those listed previously with the nucleated cavities having radius, $R = 1.95 \times 10^{-4}$ mm and dihedral angle, $\Psi = 120^\circ$. The value of $l_{en}$ is $4.87 \times 10^{-5}$ mm. The nucleation rate used was $N = 1.03 \times 10^{-3}$ s$^{-1}$. There is significant amount of cavity coalescence at the later stages of the simulation. This is due to the large number of cavities present on the grain boundary (the peak number was 125), this number had reduced to 37 at the critical damage fraction.

Figure 135. Off-centre cavity evolution for applied stress of 20 MPa and $M_a/M_{gb} = 1$.

Due to the slow surface diffusion the cavities remain 'crack-like' in shape. As in the earlier cases of pre-existing cavities those which are furthest from the large 'crack-like' cavity tend to grow the most and form another 'mini-crack', this is accentuated by the off-centre load that produces the highest tension at the left hand end. At the final critical
damage fraction the large 'crack-like' cavity had extended in length by 1.9%. The 'opening-up' of the grain boundary can also cause the cavities to 'shift' along the grain boundary using the $\dot{x}_c$ degree of freedom. It can be seen that the large 'crack-like' cavity does not move by any significant amount. The smaller cavities do tend to move towards the opening end of the grain boundary but by only relatively small amounts. The actual amounts are difficult to measure, as when there is coalescence the position of the new cavity centre is different to the original. There is very limited growth to the right of the 'crack-like' cavity, this is due to the compression of the grain boundary due to the rotation.

**Case 10:** $\sigma_{av} = 20$ MPa, $M_s = 2.08 \times 10^{-15}$, $M_{gb} = 2.08 \times 10^{-17}$, $M_s/M_{gb} = 100$.

Figure 136 shows the evolution for an averaged applied stress of 20 MPa and a ratio of $M_s/M_{gb} = 100$.

![Diagram of cavity evolution](image)

Figure 136. Off-centre cavity evolution for applied stress of 20 MPa and $M_s/M_{gb} = 100$. 
This simulation uses the same material and simulation parameters as the previous case as well as the nucleation rate $\dot{N}$. The nucleating cavities can be seen from an earlier stage in this case than in case 9, as the fast surface diffusion allows them to remain more spherical. It can be seen that there is a significant amount of coalescence towards the latter stages of the simulation and the size and number of cavities remaining reduces drastically. There were 78 cavities present at the peak and this reduced to just 24 at the critical damage fraction. At this final damage fraction the large ‘crack-like’ cavity had grown in length by 20% compared to its initial length. As in the previous case the cavities tended to ‘shift’ towards the opening side of the grain boundary and the large ‘crack-like’ cavity centre moved by $6 \times 10^{-3}$ mm to the left. Again, it can be seen that there is very limited growth to the right of the ‘crack-like’ cavity due to the compression of the grain boundary.

**Case 11: $\sigma_{av} = 200$ MPa, $M_g = 2.08 \times 10^{-17}, M_{gb} = 2.08 \times 10^{-17}, M_g/M_{gb}=1$.**

Figure 137 shows the evolution for an averaged applied stress of 200 MPa and a ratio of $M_g/M_{gb} = 1$. The main material and simulation parameters used in this case are the same as those in the previous case.

![Diagram](image-url)

**Figure 137. Off-centre cavity evolution for applied stress of 200 MPa and $M_g/M_{gb}=1$.**
The newly nucleated cavities had radius, \( R = 8.63 \times 10^{-5} \) mm and dihedral angle, \( \Psi = 120^\circ \). The value of \( l_{\text{crit}} \) is \( 2.16 \times 10^{-5} \) mm. The nucleation rate used was \( \dot{N} = 1.03 \times 10^{-3} \) s\(^{-1} \). As expected the nucleated cavities remain too small to be seen on the grain boundary although there is a significant amount of growth occurring. There were 120 cavities present at the peak and at the critical damage fraction the number of cavities present had reduced to just 11. This is shown in the figure by the large ‘crack-like’ cavity occupying the majority of the grain boundary at the 90% damage fraction.

It can be seen from the Figure 137 that the majority of the coalescence occurred between the 80 and 90% damage fractions. This is a very late stage in the lifetime and it is possible that if this were a real material it would have failed before reaching 90%. The figure shows that the large ‘crack-like’ cavity has propagated along the grain boundary and at the final damage fraction it had increased in length by 322%. This is partly due to the high stress and slow surface diffusion but also due to the off-centred load that is effectively ‘squeezing’ the cavity from the right hand side and making it move to the left. The random nucleation causes local damage, which grows rapidly and then coalesces with the large cavity allowing it to continue growing.

As in previous cases the cavities tended to ‘shift’ towards the opening end of the grain boundary although these are difficult to see in the figure. The centre of the large ‘crack-like’ cavity has ‘shifted’ by \( 5.49 \times 10^{-2} \) mm to the left, although this is mainly due to coalescence with the smaller cavities.

**Case 12:** \( \sigma_{\text{av}} = 200 \) MPa, \( M_g = 2.08 \times 10^{-15} \), \( M_{gb} = 2.08 \times 10^{-17} \), \( M_g/M_{gb} = 100 \).

The final case presented here is for an averaged applied stress of 200 MPa and a ratio of \( M_g/M_{gb} = 100 \), it is shown in Figure 138. This case uses the same material and simulation parameters as those used in the previous case except for the increased \( M_g/M_{gb} \). As in case 10, the nucleated cavities can be seen on the grain boundary at an earlier stage than those in case 11. In this simulation there were 85 cavities at the peak, with the number falling to 67 at the final damage fraction due to coalescence. Figure 138 shows that there was not as much coalescence as in the previous case although the peak number of cavities was similar to that in case 10. This could be due to the positions of the cavities and the fact that they
were not nucleated in positions that were close enough to other cavities to allow them to coalesce.

\[
\begin{align*}
& t = 0, \text{27\% damage} \\
& t = 7.4\times10^4\text{s}, \text{60\% damage} \\
& t = 7.95\times10^4\text{s}, \text{70\% damage} \\
& t = 8.14\times10^4\text{s}, \text{80\% damage} \\
& t = 8.22\times10^4\text{s}, \text{90\% damage}
\end{align*}
\]

**Figure 138. Off-centre cavity evolution for applied stress of 200 MPa and \( \frac{M_s}{M_{gb}}=100 \).**

At the critical damage fraction the large ‘crack-like cavity’ had extended in length by 1.5\%. This is significantly less than the 20\% extension from case 10, which also had fast surface diffusion. As in the three previous cases the smaller cavities tended to ‘shift’ towards the opening end of the grain boundary. The amount the large ‘crack-like’ cavity moved to the left was very small \( (1\times10^{-5} \text{ mm}) \). Unlike cases 9 and 10 there has been a significant amount of growth to the right of the ‘crack-like’ cavity. In this case the increased load and separation rate allow the cavities to grow larger than in the previous cases.
8.4 Conclusions.

The presence of a large cavity on the grain boundary reduces the effective grain boundary area that carries the applied load. This results in a higher local stress along the remaining grain boundary. Cavities subsequently nucleated on the remaining grain boundary ‘feel’ the effect of the large ‘crack-like’ cavity in this way. The numerical simulations presented in this chapter suggest that this appears to be the only way in which the large ‘crack-like’ cavity interacts with the smaller cavities. In almost all the cases the large ‘crack-like’ cavity never propagates through the smaller cavities by coalescing with them. The smaller cavities grow almost independently once nucleated, this leads to an almost ‘uniform’ debounding of the grain boundary. This is even the case when an off-centred load is applied and the grains are allowed to rotate. The inclusion of continuous nucleation also does not alter this conclusion.

The set of cases with pre-existing cavities on the grain boundary highlighted the formation of the mini-cracks that then continued to grow independently. The cases with fast surface diffusion showed the cavities maintaining a more spherical shape throughout the evolution. The applied stress of 200 MPa produced the largest crack growth with total coalescence and only the crack remaining at the critical damage fraction.

The set of cases without the pre-existing cavities but with continuous random nucleation showed that the fast surface diffusion cases tended to produce the larger cavities, which were clearly seen on the grain boundary. The slower surface diffusion cases produced very thin ‘crack-like’ cavities, which did not appear in the plots of the system. In all of the cases there was very little crack propagation with the maximum amount being 3.1%. The results from these simulations confirmed the results of Pan and Cocks, (2000), in that the majority of damage accumulation comes from the growth of the cavities as opposed to the propagation of the crack through the material.

The final set of cases discussed had an off-centred load and large ‘crack-like’ cavity with continuous random nucleation. The results produced were more mixed. The cases with slow surface diffusion tended to coalesce more to form larger cavities. This was shown in the extreme by case 11 in which the large ‘crack-like’ cavity grew by 322%. Whereas the
Chapter 8 Large 'crack-like' cavity evolution.

cases with fast surface diffusion tended to have less coalescence. Despite this, case 10 showed an increase in the large 'crack-like' cavity length of 20%.

In the case of the results by Pan and Cocks, (2000), Figure 120 shows that the cavities that are placed ahead of the crack all grow at very similar rates. Those nearest the crack tip grow slightly faster than those further away, however they are soon caught up in terms of size. It can also be seen that there is only a small amount of crack propagation from the initial figure to the final one, it is approximately 30% longer than the initial stage.

One of the main reasons we are not observing a stress concentration is because elasticity is neglected. The simplified finite element model assumes the grains are rigid and as such they move apart in a uniform manner without elastic effects. The justification for this is that the time frame for elasticity effects is very small compared to that for the creep damage. In effect, it is the 'steady-state' stress state that is being seen, i.e. one in which the instantaneous effects of elasticity have 'relaxed' to form the type of stress distribution observed in the results. This explains the absence of an asymptotic stress value ahead of the crack tip; instead it has reduced to form the parabolic stress distribution as shown in Figure 124 and Figure 125.

It remains unclear if these predictions from the 'steady-state' diffusional damage model agree with the actual observations for an engineering alloy. It is well established that a macroscopic crack does propagate through the material leading to the final failure of a component. At the microscopic level however, the evidence is less clear. It was not possible to obtain any direct experimental evidence from the literature that either supports or contradicts these predictions.

The numerical studies in this work serve two purposes, (a) if experimental evidence can be obtained to contradict the predictions, then this work suggests the 'steady-state' diffusional cavity growth model is not good enough to capture the real material behaviour. (b) in the absence of confirmation from experimental results, it remains a possibility that the interaction between large and small cavities is weak and can be ignored, except for the load transfer effect. If confirmed by the experimental evidence, this has profound implications on the further modelling of the creep damage evolution on a larger scale, since it would significantly simplify the modelling task.
9. Concluding remarks and future work.

In this work a simplified single cavity growth model incorporating the effects of grain boundary and surface diffusion has been developed. This model was then validated using the full finite element model developed by Pan et al., (1997). Upon validation, the model was extended to simulate multiple cavities on a grain boundary using the classical finite element approach. This simplified finite element model is also able to model continuous nucleation and cavity coalescence. Using the simplified finite element model the effects of surface diffusion on creep life were investigated. It was also compared with the ‘smeared-out’ model by Nguyen et al., (1998). Finally, this simplified model was used to simulate the evolution of large ‘crack-like’ cavities on a grain boundary.

In this chapter a brief review of the key achievements is given and the possible areas for the continuation of this research are suggested based on the conclusions drawn throughout the work.

9.1 Major achievements in this work.

A review of the existing literature in the area of diffusional creep damage accumulation identified the need to develop a new simplified diffusional creep model, which was able to simulate the evolution of multiple cavities on the grain boundary without requiring large amounts of processing time. It was shown that the phenomenon of creep is not a new one and that it has great importance in industries that use high temperature plant. The models currently in use were discussed in chapter 3.

The use of full finite element models to simulate the evolution of a single cavity was discussed in chapter 3 with the main drawback being the complexity of such a model and the difficulty in extending it to model multiple cavities. In chapter 4 a new simplified model using only 2 degrees of freedom was constructed to simulate the evolution of a single cavity on a grain boundary by coupled surface and grain boundary diffusion. The new model is relatively simple compared to the full finite element model and was found to require only a fraction of the processing time compared to that of the full finite element
model. It was shown to give excellent agreement with the full finite element model under practical material and loading conditions. Conventional methods state that the assumption of an arc with constant curvature would result in no flux being produced. However, the use of the variational principle allows the so-called weak solution to be used when deriving the chemical potential expressions. This releases the relationship between the chemical potential and the curvature. The results from the simplified finite element model demonstrated the validity of the weak solution technique. The new simplified model was also simple enough to be extended to simulate the evolution of multiple cavities on the grain boundary and this is discussed below.

Using the simplified 2 degree of freedom model defined in chapter 4 the work moved on to extending it to simulate multiple cavities using the classical finite element approach for element assembly. This new simplified finite element model outlined in chapter 5 was shown to be able to simulate a large number of cavities (350 was the maximum number tested). Continuous cavity nucleation was included in the model as well as cavity coalescence. One of the main advantages of the simplified finite element model was the processing time required to complete a simulation. Even with 200 cavities on the grain boundary the majority of the simulations took less than 24 hours to complete. This model can also be used to simulate a wide range of systems such the pre-existence of cavities, which can be large and ‘crack-like’ or small and spherical in shape.

In chapter 6 the ‘smeared-out’ model by Nguyen et al., (1998) was discussed and compared with the simplified multi-cavity finite element model. The relatively simple ‘smeared-out’ model required even less processing time than the simplified multiple cavity model, with simulations taking in the order of 1-2 minutes to complete. In this model there were no discrete cavities and the assumption was made that they were uniform in size and distribution. This assumption has been shown to be inappropriate as the results from the simplified finite element model showed a wide variation in cavity sizes and separations from the initial stages of the simulations. The ‘smeared-out’ model also could not model the interaction between the cavities. When continuous nucleation was included in the ‘smeared-out’ model it significantly under-predicted the lifetime of the grain boundary. This was due to the assumption of the uniform cavities, as the size of the newly nucleated cavity has to be the same size as the existing cavities on the grain boundary at the time of nucleation. The model therefore nucleates larger and larger cavities, whereas
in reality the nucleated cavities should be very small. It was further shown that the ‘smeared-out’ model only agrees with the simplified finite element model at very unrealistic conditions such as very high applied stresses or very low nucleation rates.

Chapter 7 investigated the effects of surface diffusion on the creep life. It was shown in chapter 4 how surface diffusion affects the shape of a single cavity during the evolution and this was repeated for multiple cavities on a single grain boundary. The results clearly showed the cavities evolving to thin ‘crack-like’ cavities under high applied stresses or when the surface diffusion was slow. And, consequently the cavities tended to stay more spherical for fast surface diffusion or low applied stress cases. This provided confirmation that the simplified finite element model was working correctly. The effects of surface diffusion on the rupture time are also shown. In the majority of the cases the rupture time increased as the surface diffusion increased, this result is another confirmation of the results from the simplified cavity model in chapter 4. However, at lower applied stresses (typically ≤ 35MPa), the effect of surface diffusion on the creep life was reversed, i.e. the faster the surface diffusion the shorter the rupture time.

The final chapter investigated the evolution of a large pre-existing ‘crack-like’ cavity and whether it was possible to simulate the propagation of the ‘crack-like’ cavity along the grain boundary. In this case a large thin ‘crack-like’ cavity was placed on the grain boundary. Several different scenarios were investigated such as: pre-existing smaller cavities in front of the large ‘crack-like’ cavity, no existing cavities but instead continuous nucleation of cavities, and finally asymmetric loads and cavities. The results from the simplified finite element model showed that on a single grain boundary the local stress did not reach a sufficiently high value to cause the crack-like cavity to propagate. Instead the smaller cavities tended to grow independently of the large ‘crack-like’ cavity and only coalesce towards the very end of the creep life. These results were in agreement with the non-published results of Pan et al., (private communication), who also showed that the creep life was controlled by the growth and coalescence of the smaller cavities.
9.2 Future work.

The development of the simplified finite element model simulates the evolution of multiple cavities on a single grain boundary without requiring excessive amounts of processing time. However, there are still some limitations and problems which have been encountered and areas of possible future work are suggested based on these.

Five areas of further developments are outlined in this section.

- At present the model can only simulate the evolution of cavities on a single grain boundary. The next stage of the work could investigate extending the simplified finite element model to simulate the evolution of a number of grain boundaries connected together to form a grain. This would increase the application of the model, as it would increase the fraction of material that could be simulated, thus providing a more realistic projection of creep life.

- Once the model had been extended to simulate the evolution of whole grains it could be embedded into a continuum finite element model such as the one developed by Pan et al. Such a new model could then be used to predict the cavity growth and crack propagation within a representative element of an engineering material.

- The modelling of inclusions could be incorporated into the simplified finite element model. These are known to effect the progress of the creep process as well as being prime sites for the nucleation of cavities.

- The mechanisms of plasticity and power-law creep could be included in the model. The inclusion of these mechanisms would give the model a wider range of applicability. If we refer to the deformation mechanism map shown in Figure 6 it can be seen that these mechanisms operate at higher temperatures and stresses than those currently modelled with the diffusional mechanisms.
- The simplified finite element model could be extended to three dimensions. This would require a very large amount of additional research, and the processing demands would also be very considerable. However, the three dimensional model would provide a more complete simulation of how the cavities evolved on the grain boundary.
References.


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Appendix A - Cavity surface migration velocity.

This section describes how a unit vector is used to derive the expressions for the cavity surface migration velocity. Using Figure 26, we say that:

\[ n_x = -\sin \theta \quad \text{and} \quad n_y = -\cos \theta \quad (A-1) \]

Where \((n_x, n_y)\) is the unit vector normal to the cavity surface pointing out of the material. The reason for the negative signs are due to the fact that we are dealing with a cavity, it is normal in these circumstances to move from the material into the void. This means that the displacements are negative according to the origin. The negative signs are used to represent this. Therefore:

\[ \dot{X} = V_s \sin \theta \quad \text{and} \quad \dot{Y} = V_s \cos \theta \]

Then

\[ \dot{X} + \dot{Y} = V_s(\sin \theta + \cos \theta) \]
\[ X^2 + Y^2 = V_s^2(\sin^2 \theta + \cos^2 \theta) \]
\[ V_s = \sqrt{X^2 + Y^2} \quad (A-2) \]

In order to show that this expression is correct, there follows a short proof:

Using simple trigonometry we can say that:

\[ \cos \theta = \frac{\dot{Y}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} \quad \& \quad \sin \theta = \frac{\dot{X}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} \quad (A-3) \]

\[ n_y = \frac{\dot{Y}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} \quad \& \quad n_x = \frac{\dot{X}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} \quad (A-4) \]

Using Equation (4.3-12), we know that:

\[ V_s = \dot{X} n_x + \dot{Y} n_y \quad (A-5) \]

Substituting (A-4) into (A-5) we arrive at:

\[ V_s = \frac{\dot{X}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} + \frac{\dot{Y}}{\sqrt{\dot{X}^2 + \dot{Y}^2}} \]
Therefore the expression derived for the cavity surface migration velocity has been proved to be valid.
Appendix B – 2 degree of freedom model derivation.

Free energy change rate derivation.

Taking the time derivative of Equation (4.2-1), the free energy change rate can be derived as:

\[
G = \Psi R \gamma_s + (L_0 - R \sin \frac{\Psi}{2}) \gamma_{gb} - \sigma L_0 B
\]

\[
\dot{G} = \gamma_s (\dot{\Psi} R + \dot{\Psi} \dot{R}) + \gamma_{gb} \left( - \dot{R} \sin \frac{\Psi}{2} - \frac{R \dot{\Psi}}{2} \cos \frac{\Psi}{2} \right) - \sigma L_0 \dot{B}
\]

\[
\dot{G} = \left[ \gamma_s \Psi - \gamma_{gb} \sin \frac{\Psi}{2} \right] \dot{R} + \left[ \gamma_s R - \gamma_{gb} \frac{R \cos \frac{\Psi}{2}}{2} \right] \dot{\Psi} - \sigma L_0 \dot{V}_{gb} \tag{B-1}
\]

Re-writing Equation (4.3-20) and then inserting it with Equation (4.3-17) into (B-1), we obtain the final expression for the free energy change rate: i.e.

\[
\Psi = 2 \arccos \left( \frac{\gamma_{gb}}{2 \gamma_s} \right) \Rightarrow \gamma_{gb} = 2 \gamma_s \cos \left( \frac{\Psi_s}{2} \right)
\]

Hence:

\[
\dot{G} = \left[ \Psi \gamma_s - 2 \gamma_s \cos \frac{\Psi_s}{2} \sin \frac{\Psi_s}{2} \right] \dot{R} + \left[ R \gamma_s - R \gamma_s \cos \frac{\Psi_s}{2} \cos \frac{\Psi_s}{2} \right] \dot{\Psi} - \sigma L_0 \dot{V}_n
\]

\[
\dot{G} = \gamma_s \left[ \Psi - 2 \cos \frac{\Psi_s}{2} \sin \frac{\Psi_s}{2} \right] \dot{R} + \gamma_s R \left[ 1 - \cos \frac{\Psi_s}{2} \cos \frac{\Psi_s}{2} \right] \dot{\Psi}
\]

\[
- \frac{\sigma \alpha L_0}{L_0 - R \sin \Psi} \left[ R \dot{R} (\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \dot{\Psi} \right] \tag{B-2}
\]
Surface term derivation.

The surface flux expression can be obtained using (A-1) and integrating the matter conservation expression (4.2-12) as follows:

\[
X = R \sin \theta \\
\dot{X} = \dot{R} \sin \theta \\
Y = R \cos \theta - C = R \cos \theta - R \cos \frac{\Psi}{2} \\
\dot{Y} = \dot{R} \cos \theta - \dot{R} \cos \frac{\Psi}{2} + \frac{R}{2} \sin \frac{\Psi}{2} \dot{\Psi} 
\]

(B-3)

(B-4)

Now multiplying by the unit vectors, we have:

\[
\dot{X}n_x = \dot{R} \sin \theta (\sin \theta) = -\dot{R} \sin^2 \theta 
\]

(B-5)

\[
\dot{Y}n_y = \left( \dot{R} \cos \theta - \dot{R} \cos \frac{\Psi}{2} + \frac{R}{2} \sin \frac{\Psi}{2} \dot{\Psi} \right) (\cos \theta) \\
\dot{Y}n_y = -\dot{R} \cos^2 \theta + \dot{R} \cos \theta \cos \frac{\Psi}{2} - \frac{R}{2} \cos \theta \sin \frac{\Psi}{2} \dot{\Psi} 
\]

(B-6)

Using (4.3-13), the expression for \( V_x \) now becomes:

\[
V_x = -\dot{R} \sin^2 \theta - \dot{R} \cos^2 \theta + \dot{R} \cos \theta \cos \frac{\Psi}{2} - \frac{R}{2} \cos \theta \sin \frac{\Psi}{2} \dot{\Psi} \\
- V_x = \dot{R} (\sin^2 \theta + \cos^2 \theta) - \dot{R} \cos \theta \cos \frac{\Psi}{2} + \frac{R}{2} \cos \theta \sin \frac{\Psi}{2} \dot{\Psi} \\
- V_x = \dot{R} - \dot{R} \cos \theta \cos \frac{\Psi}{2} + \frac{R}{2} \cos \theta \sin \frac{\Psi}{2} \dot{\Psi} 
\]

(B-7)

Now using the matter conservation expression (4.2-12):

\[
V_x + \frac{\partial J_x}{\partial \xi} = 0 \quad \Rightarrow \quad J_x = \int_{r_x}^{R} \left( -V_x \right) \, d\xi 
\]

\( V_x \) is a function of \( \theta \), therefore we change the variable using:
\[ \dot{s} = R \cdot \partial \theta \quad \therefore \quad J_s = \int_{r_i} -V_s(\theta), R \partial \theta \]  

(B-8)

Now inserting (B-7) into (B-8), we arrive at the expression for the surface flux:

\[
\begin{align*}
J_s &= R \int_{r_i} \left[ \dot{R} - \dot{R}' \cos \theta \cos \frac{\Psi}{2} + \frac{R}{2} \cos \theta \sin \frac{\Psi}{2}, \dot{\Psi} \right] d\theta \\
J_s &= R \dot{R} \theta - \dot{R} \sin \theta \cos \frac{\Psi}{2} + \frac{R}{2} \sin \theta \sin \frac{\Psi}{2}, \dot{\Psi} \\
J_s &= R \dot{R} \left[ \theta - \cos \frac{\Psi}{2} \sin \theta \right] + \frac{R^2}{2} \sin \frac{\Psi}{2} \sin \theta, \dot{\Psi}  
\end{align*}
\]  

(B-9)

The surface term can be evaluated using Equation 4.3-14 as shown below:

\[
\int \frac{J^2}{2M_s} dS = \frac{R^2}{2M_s} \int_{r_i} \left[ \left( \theta - \cos \frac{\Psi}{2} \sin \theta \right) + \frac{R}{2} \sin \frac{\Psi}{2} \dot{\Psi} \right]^2 d\theta \\
= \frac{R^2}{2M_s} \left[ \frac{\dot{R}^2}{24} \cos^2 \frac{\Psi}{2} \left[ \left( 2 + \cos \frac{\Psi}{2} - \sin \frac{\Psi}{2} \right) + \frac{R^2}{4} \cos \frac{\Psi}{2} \sin \frac{\Psi}{2} \left( 1 - \sin \Psi \right) \right] \\
+ \frac{R^2}{16} \sin^2 \frac{\Psi}{2} \dot{\Psi}^2 \left( 1 - \cos \Psi \right) \right] \\
\frac{R^2}{2M_s} \right]
\]

Re-writing, using double angle formulae, we have:

\[
\begin{align*}
\frac{\dot{R}^2}{24} + \frac{\dot{R}^2}{2} \left[ \Psi + \Psi \cos \Psi - 2 \sin \Psi \right] + \frac{\dot{R} \Psi}{4} \left[ \frac{\Psi}{2} - \frac{1}{2} \cos \Psi \right] \\
= \frac{\dot{R}^2}{8} \left[ \Psi - \sin \Psi + \Psi \cos \Psi - \frac{1}{2} \sin 2\Psi \right] - \frac{\dot{R} \Psi}{8} \left[ \frac{\Psi}{8} - \frac{1}{16} + \frac{1}{16} \cos 2\Psi \right] \\
+ \frac{R^2}{16} \left[ \Psi - \sin \Psi \right] \left( 1 - \cos \Psi \right) \\
\frac{R^2}{2M_s} \right]
\]

Finally, Collecting terms of \( \dot{R}^2 \), \( \dot{R} \Psi \) & \( \dot{\Psi}^2 \) respectively:

\[
\begin{align*}
= \dot{R}^2 \frac{\Psi^3}{24} + \dot{R}^2 \left[ \frac{\Psi}{2} + \frac{\Psi \cos \Psi}{2} - \sin \Psi \right] + \dot{R}^2 \left[ \frac{\Psi}{8} - \frac{\Psi}{8} + \frac{\Psi \cos \Psi}{8} - \frac{\sin 2\Psi}{16} \right] \\
= \dot{R}^2 \left[ \frac{5\Psi}{8} + \frac{5\Psi \cos \Psi}{8} - \frac{9 \sin \Psi}{8} - \frac{\sin 2\Psi}{16} + \frac{\Psi^3}{24} \right] \frac{R^2}{2M_s} \\
\]

\]
Equations (B-10.1), (B-10.2) & (B-10.3) are recombined into one expression, which gives the evaluated surface term. We also remember that there are two free surfaces in the model, therefore the entire expression is multiplied by a factor of two.

**Grain boundary term derivation.**

The grain boundary separation velocity ($V_{gb}$), is assumed to be constant along the length of grain boundary. The grain boundary flux expression can be obtained by integrating the matter conservation expression (4.2-13) as follows:

\[
V_{gb} + \frac{\partial J_{gb}}{\partial X} = 0
\]

\[
V_{gb} + \frac{\partial J_{gb}}{\partial X} = 0 \quad \Rightarrow \quad J_{gb} = \int V_{gb} \partial X
\]

\[
J_{gb} = -V_{gb}X + C
\]  

(B-11)

Using boundary conditions of:

@ $X = L_a$ then $J_{gb} = 0$
We have:
\[ 0 = -V_{gb}L_0 + C \quad \Rightarrow \quad C = V_{gb}L_0 \]  
(B-12)

Therefore, combining (B-11) and (B-12):
\[ J_{gb} = V_{gb}(L_0 - X) \]  
(B-13)

If matter conservation is to be satisfied then, at the point the grain boundary meets the cavity surface, the following must be true:
\[ \left( J_{gb} \right)_{x=L_0} = 2 \left( J_s \right)_{\theta = \frac{\Psi}{2}} \]  
(B-14)

\[ X = L_1 = R \sin \frac{\Psi}{2} \]

\[ J_{gb} = V_{gb} \left( L_0 - R \sin \frac{\Psi}{2} \right) \]  
(B-15)

Using the surface flux expression (B-9) at \( \theta = \frac{\Psi}{2} \), we have:
\[ 2J_s = 2R \left( \frac{R}{2} - \cos \frac{\Psi}{2} \sin \frac{\Psi}{2} \right) + R^2 \sin \frac{\Psi}{2} \sin \frac{\Psi}{2} \Psi \]

The expression reduces to:
\[ 2J_s = R \left[ \Psi - \sin \Psi \right] + \frac{R^2}{2} [1 - \cos \Psi], \Psi \]  
(B-16)

Equating (B-15) with (B-16), we arrive at the expression for the grain boundary flux:
\[ V_{gb} \left( L_0 - R \sin \frac{\Psi}{2} \right) = R \left[ \Psi - \sin \Psi \right] + \frac{R^2}{2} [1 - \cos \Psi], \Psi \]

\[ V_{gb} = \frac{1}{\left( L_0 - R \sin \frac{\Psi}{2} \right)} R \left[ \Psi - \sin \Psi \right] + \frac{R^2}{2} [1 - \cos \Psi], \Psi \]

\[ J_{gb} = \frac{L_0 - X}{L_0 - R \sin \frac{\Psi}{2}} \left[ R \left[ \Psi - \sin \Psi \right] + \frac{R^2}{2} [1 - \cos \Psi], \Psi \right] \]  
(B-17)
The grain boundary term can be evaluated using Equation 4.3-18:

\[
\int J_{gb}^2 \frac{dX}{2M_{gb}} = \int L_t J_{gb}^2 \frac{dX}{2M_{gb}}
\]

\[
= \int L_t \frac{1}{2M_{gb}} \left( \frac{L_0 - X}{L_0 - R \sin \frac{\Psi}{2}} \left[ R \hat{R}(\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \Psi \right] \right) dX
\]

\[
= \frac{1}{2M_{gb}} \left( \frac{L_0 - R \sin \frac{\Psi}{2}}{2} \right)^3 \left[ R \hat{R}(\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \Psi \right]^2 \int L_t \left( \frac{L_0 - X}{3} \right) dX
\]

\[
= \frac{\left( \frac{L_0 - R \sin \frac{\Psi}{2}}{2} \right)^3}{6M_{gb}^2} \left[ R \hat{R}(\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \Psi \right]^2 \left( \frac{L_0 - X}{3} \right) \int L_t
\]

\[
= \frac{1}{6M_{gb}^2} \left( \frac{L_0 - R \sin \frac{\Psi}{2}}{2} \right)^3 \left[ R \hat{R}(\Psi - \sin \Psi) + \frac{R^2}{2} (1 - \cos \Psi) \Psi \right]^2
\]

\[
(B-18)
\]

Energy dissipation due to grain boundary opening.

The extra free energy dissipation related to the opening of junction can be derived using Figure 27. By simple geometry, it can be seen that:

\[
\sin \left( \frac{\Psi}{2} \right) = \frac{V_{gb}}{2} \Rightarrow \frac{1}{2} \Delta S_f \sin \left( \frac{\Psi}{2} \right) = \frac{V_{gb}}{2}
\]

As we are considering only half of the system we multiply by two:

\[
\Delta S_f = \frac{V_{gb}}{2} \frac{\Psi}{\sin \frac{\Psi}{2}}
\]
For the change in the grain boundary length:

\[
\tan \left( \frac{\Psi}{2} \right) = \frac{\left( \frac{V_{gb}}{2} \right)}{\Delta S_{gb}} \Rightarrow \Delta S_{gb} = \frac{\left( \frac{V_{gb}}{2} \right)}{\tan \left( \frac{\Psi}{2} \right)} = \frac{V_{gb}}{2} \left( \frac{\cos \left( \frac{\Psi}{2} \right)}{\sin \left( \frac{\Psi}{2} \right)} \right)
\]

The changes in length can now be used to calculate the rate of change of energy for the opening of the grain boundary:

\[
\frac{dE}{dt} = \Delta S_f \cdot \gamma_s - \Delta S_{gb} \cdot \gamma_{gb}
\]

\[
\frac{dE}{dt} = \frac{V_{gb}}{\sin \left( \frac{\Psi}{2} \right)} \cdot \frac{\cos \left( \frac{\Psi}{2} \right)}{\sin \left( \frac{\Psi}{2} \right)} \gamma_{gb}
\]

\[
\frac{dE}{dt} = V_{gb} \left( \frac{\gamma_s}{\sin \left( \frac{\Psi}{2} \right)} - \frac{\gamma_{gb}}{2 \tan \left( \frac{\Psi}{2} \right)} \right) = \dot{G}_{\text{junction}}
\]

\[
\dot{G}_{\text{junction}} = \left[ \frac{\gamma_s}{\sin \left( \frac{\Psi}{2} \right)} - \frac{\gamma_{gb}}{2 \tan \left( \frac{\Psi}{2} \right)} \right] \left[ \frac{R R(\Psi - \sin \Psi) + \frac{R^2}{2}(1 - \cos \Psi)\Psi}{L_0 - R \sin \left( \frac{\Psi}{2} \right)} \right]
\]

**Classification of variables.**

In order to reduce the amount of characters quoted in the final expressions we define the following variables that represent various parts of the full equations:

\[
A_1 = 5\Psi + 5\Psi \cos \Psi + \frac{1}{3} \Psi^3 - 9\sin \Psi - \frac{1}{2} \sin 2\Psi
\]

\[
A_2 = 9 - 8 \cos \Psi - 6\Psi \sin \Psi - \cos 2\Psi
\]

\[
A_3 = \frac{4}{3} \frac{M_s}{M_{gb}} \left( 1 - \frac{R}{L_0} \sin \frac{\Psi}{2} \right)
\]

\[
A_4 = \Psi - \sin \Psi
\]

\[
A_5 = 1 - \frac{R}{L_0} \sin \frac{\Psi}{2}
\]
\[ A_6 = \Psi - 2 \cos \frac{\Psi}{2} \sin \frac{\Psi}{2} \]
\[ A_7 = 1 - \cos \frac{\Psi}{2} \cos \frac{\Psi}{2} \]
\[ A_8 = 1 - \cos \Psi \]

These variables are now inserted into the following Equations:

- (B-2) - Free energy change rate expression
- (B-10.1) - Surface flux term
- (B-10.2) - Grain boundary flux term
- (B-10.3) - Extra term for grain boundary opening

Hence the expressions are now written as:

(B-2) becomes:
\[ \dot{G} = \gamma_s A_6 \dot{R} + \gamma_s A_4 R \dot{\Psi} - \frac{\sigma_{es}}{A_2} \left[ A_4 R \dot{R} + \frac{A_8 R^2}{2} \dot{\Psi} \right] \]

(B-10) becomes:
\[ \int_{2 M_s}^{\psi_2} \frac{J^2}{2 M_s} dS = \frac{A_4 R^2 \dot{R}^2}{8 M_s} + \frac{A_2 R^3 \dot{R} \dot{\Psi}}{16 M_s} + \frac{A_4 A_5 R^4 \dot{\Psi}^2}{32 M_s} \]

(B-18) becomes:
\[ \int_{g_b}^{2 M_{gb}} \frac{J^2}{2 M_{gb}} dX = \frac{A_5 L_0}{6 M_{gb}} \left[ A_4 R \dot{R} + \frac{A_8 R^2 \dot{\Psi}}{2} \right] \]

(B-19) becomes:
\[ \dot{G}_{junc} = \frac{A_7 \gamma_s}{A_5 L_0 \sin \frac{\Psi}{2}} \left[ A_4 R \dot{R} + \frac{A_8 R^2 \dot{\Psi}}{2} \right] \]

We now collect terms of \( \dot{R}^2, \dot{R} \dot{\Psi}, \dot{\Psi}^2, \dot{R} \& \dot{\Psi} \) respectively:

\[ A_{RR} = \frac{A_4 R^2}{4 M_s} + \frac{A_5 A_4 L_0 R^2}{3 M_{gb}} \]
(B-20)
\[ A_{R\Psi} = \frac{A_2 R^3}{16 M_s} + \frac{A_4 A_5 A_8 L_0 R^2}{6 M_{gb}} \]
(B-21)
\[ A_{\Psi\Psi} = \frac{A_4 A_5 R^4}{16 M_s} + \frac{A_5 A_8 L_0 R^4}{12 M_{gb}} \]
(B-22)
Using Equation (4.3-10), we obtain the two ordinary differential equations, which govern the evolution of the cavities, these are shown below:

\[
\frac{\partial \Theta}{\partial R} = \left[ \frac{A_1 R^2}{4 M_s} + \frac{A_2 A_4 L_0 R^2}{6 M_{gb}} \right] \dot{R} + \left[ \frac{A_3 R^3}{16 M_s} + \frac{A_4 A_5 A_7 L_0 R^3}{6 M_{gb}} \right] \dot{\psi} = \left[ \frac{A_4 \sigma_{xz}}{A_5} - \frac{A_4 A_7 R}{A_5 L_0 \sin \frac{\psi}{2}} - A_6 \right] \tag{B-25}
\]

\[
\frac{\partial \Theta}{\partial \psi} = \frac{A_2 R^3}{16 M_s} + \frac{A_4 A_5 A_7 L_0 R^3}{12 M_{gb}} \dot{R} + \left[ \frac{A_3 A_4 R^4}{16 M_s} + \frac{A_4 A_5^2 L_0 R^3}{12 M_{gb}} \right] \dot{\psi} = \left[ \frac{A_8 R^2 \sigma_{xz}}{2 A_5} - \frac{A_7 A_8 R^2}{2 A_5 L_0 \sin \frac{\psi}{2}} - A_9 \right] \tag{B-26}
\]

These are now inserted into (4.3-23) and can be solved using the methods outlined in previous sections.
Appendix C – Materials Data.

The following table gives actual material values for the ratio of mobilities at two fractions of the melting temperatures ($T_{melt}$). These are $0.5T_{melt}$ and $0.8T_{melt}$. This data was used in the simulations as a means of demonstrating the applicability of this model to real materials.

Table C-1. Materials data for simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>Alpha-Iron</th>
<th>Alumina</th>
<th>Aluminium</th>
<th>Astrolay</th>
<th>Copper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic Volume (m$^3$/atom)</td>
<td>1.18E-29</td>
<td>1.42E-29</td>
<td>1.66E-29</td>
<td>1.08E-29</td>
<td>1.18E-29</td>
</tr>
<tr>
<td>$T_{melting}$ (K)</td>
<td>1810</td>
<td>2320</td>
<td>933</td>
<td>1673</td>
<td>1356</td>
</tr>
<tr>
<td>Pre-exp. boundary diffusion (m$^3$/s)</td>
<td>1.12E-12</td>
<td>8.60E-10</td>
<td>5.00E-14</td>
<td>2.80E-15</td>
<td>5.12E-15</td>
</tr>
<tr>
<td>Activ. Enrgy (bdry diffusion) J / mol</td>
<td>174000</td>
<td>419000</td>
<td>84000</td>
<td>115000</td>
<td>104000</td>
</tr>
<tr>
<td>Pre-exp. surface diffusion (m$^3$/s)</td>
<td>2.50E-09</td>
<td>8.60E-06</td>
<td>1.30E-11</td>
<td>1.06E-09</td>
<td>6.00E-10</td>
</tr>
<tr>
<td>Activ. Enrgy (surf diffusion) J / mol</td>
<td>232000</td>
<td>500000</td>
<td>142000</td>
<td>285000</td>
<td>204800</td>
</tr>
<tr>
<td>0.5*$T_{melt}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{gb}$*delta_gb</td>
<td>9.57E-20</td>
<td>1.03E-25</td>
<td>5.06E-20</td>
<td>1.72E-19</td>
<td>6.27E-20</td>
</tr>
<tr>
<td>$M_{gb}$ (mm$^4$/s/kg)</td>
<td>1.02E-22</td>
<td>2.62E-28</td>
<td>1.63E-27</td>
<td>1.69E-27</td>
<td>9.98E-26</td>
</tr>
<tr>
<td>$D_{s}$*delta_s</td>
<td>9.59E-20</td>
<td>2.32E-25</td>
<td>4.21E-24</td>
<td>1.58E-24</td>
<td>1.26E-22</td>
</tr>
<tr>
<td>$M_{s}$ (mm$^4$/s/kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{s}/M_{gb}$</td>
<td>1.00E+00</td>
<td>2.25E+00</td>
<td>8.33E-05</td>
<td>9.17E-06</td>
<td>2.01E-03</td>
</tr>
<tr>
<td>0.8*$T_{melt}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{gb}$*delta_gb</td>
<td>5.92E-19</td>
<td>1.39E-21</td>
<td>6.61E-20</td>
<td>9.10E-20</td>
<td>5.03E-20</td>
</tr>
<tr>
<td>$M_{gb}$ (mm$^4$/s/kg)</td>
<td>3.49E-16</td>
<td>7.68E-19</td>
<td>1.06E-16</td>
<td>5.31E-17</td>
<td>3.96E-17</td>
</tr>
<tr>
<td>$D_{s}$*delta_s</td>
<td>1.07E-17</td>
<td>7.28E-20</td>
<td>1.50E-21</td>
<td>7.98E-21</td>
<td>8.25E-20</td>
</tr>
<tr>
<td>$M_{s}$ (mm$^4$/s/kg)</td>
<td>6.30E-15</td>
<td>4.03E-17</td>
<td>2.42E-18</td>
<td>4.66E-18</td>
<td>6.50E-17</td>
</tr>
<tr>
<td>$M_{s}/M_{gb}$</td>
<td>1.80E+01</td>
<td>5.25E+01</td>
<td>2.27E-02</td>
<td>8.77E-02</td>
<td>1.64E+00</td>
</tr>
</tbody>
</table>
Table C-2. Materials data for simulations (cont.).

<table>
<thead>
<tr>
<th>Material</th>
<th>Silicon Carbide</th>
<th>Stainless Steel 304</th>
<th>Titanium Aluminide</th>
<th>Zirconia</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic Volume (m³/atom)</td>
<td>2.07E-29</td>
<td>1.21E-29</td>
<td>3.11E-29</td>
<td>1.83E-29</td>
</tr>
<tr>
<td>T_melting (K)</td>
<td>3103</td>
<td>1680</td>
<td>1730</td>
<td>2843</td>
</tr>
<tr>
<td>Pre-exp. boundary diffusion (m³/s)</td>
<td>2.20E-11</td>
<td>2.00E-13</td>
<td>7.60E-13</td>
<td>1.56E-15</td>
</tr>
<tr>
<td>Activ. Enrgy (boundary diffusion) J/mol</td>
<td>557000</td>
<td>167000</td>
<td>180000</td>
<td>286000</td>
</tr>
<tr>
<td>Pre-exp. surface diffusion (m³/s)</td>
<td>2.20E-05</td>
<td>1.10E-10</td>
<td>7.60E-10</td>
<td>1.00E-11</td>
</tr>
<tr>
<td>Activ. Enrgy (surf diffusion) J/mol</td>
<td>696000</td>
<td>220000</td>
<td>150000</td>
<td>430000</td>
</tr>
</tbody>
</table>

| 0.5* T_melt                            | 1551.5          | 840                  | 865                | 1421.5   |
| Dgb*delta_gb                           | 3.88E-30        | 8.24E-24             | 1.03E-23           | 4.82E-26 |
| Mgb (mm⁴/s/kg)                          | 3.75E-27        | 8.59E-21             | 2.67E-20           | 4.50E-23 |
| Ds*delta_s                             | 8.11E-29        | 2.29E-24             | 6.64E-19           | 1.58E-24 |
| Ms (mm⁴/s/kg)                           | 7.84E-26        | 2.39E-21             | 1.73E-15           | 1.47E-36 |

| Ms/Mgb                                  | 2.09E+01        | 2.78E-01             | 6.48E+04           | 3.28E-02 |

| 0.8* T_melt                            | 2482.4          | 1344                 | 1384               | 2274.4   |
| Dgb*delta_gb                           | 4.18E-23        | 6.46E-20             | 1.22E-19           | 4.21E-22 |
| Mgb (mm⁴/s/kg)                          | 2.53E-20        | 4.21E-17             | 1.99E-16           | 2.45E-19 |
| Ds*delta_s                             | 4.97E-20        | 3.10E-19             | 1.66E-15           | 1.33E-21 |
| Ms (mm⁴/s/kg)                           | 3.00E-17        | 2.02E-16             | 2.70E-12           | 7.75E-19 |

| Ms/Mgb                                  | 1.19E+03        | 4.79E+00             | 1.36E+04           | 3.16E+00 |

Data from: M. F. Ashby, ‘HIP 6.0 Background Reading’, Engineering Department Report, Cambridge University.

Table C-3 contains more parameters that were used in the simulations. The data is based on copper and was used by Davanas and Solomon, (1990). Copper was used as it is a material that has had a significant amount of research carried out on it. This results in there being more actual material data available for the calculation of material parameters such as diffusion coefficients. Table C-3 also shows the conversion of units from metres to millimetres, as this was the scale the simplified finite element and smeared-out models used.
### Table C-3. Material parameters for Copper.

<table>
<thead>
<tr>
<th>Constants</th>
<th>Value</th>
<th>Units</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burgers vector (b)</td>
<td>2.56E-10 m</td>
<td></td>
<td>2.56E-07 mm</td>
<td></td>
</tr>
<tr>
<td>Boltzmanns constant (k)</td>
<td>1.38E-23 J/K</td>
<td></td>
<td>1.38E-17 J/K</td>
<td></td>
</tr>
<tr>
<td>Gas Constant (R_g)</td>
<td>8.314 J/molK</td>
<td></td>
<td>8.31E+06 J/molK</td>
<td></td>
</tr>
</tbody>
</table>

#### Input Parameters

<table>
<thead>
<tr>
<th>Applied Stress</th>
<th>2.00E+07 Pa</th>
<th></th>
<th>2.00E+01 N/mm²</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp</td>
<td>1023 K</td>
<td></td>
<td>1023 K</td>
<td></td>
</tr>
<tr>
<td>Gamma_s</td>
<td>1.725 J/m²</td>
<td></td>
<td>1.73E-03 J/mm²</td>
<td></td>
</tr>
<tr>
<td>Atomic Vol. Ω</td>
<td>1.18E-29 m³</td>
<td></td>
<td>1.18E-20 mm³</td>
<td></td>
</tr>
<tr>
<td>delta_b</td>
<td>5.00E-10 m</td>
<td></td>
<td>5.00E-07 mm</td>
<td></td>
</tr>
<tr>
<td>pre_exp Db0</td>
<td>1.00E-05 m²/s</td>
<td></td>
<td>1.00E+01 mm²/s</td>
<td></td>
</tr>
<tr>
<td>pre_exp Dv0</td>
<td>7.80E-05 m²/s</td>
<td></td>
<td>7.80E+01 mm²/s</td>
<td></td>
</tr>
<tr>
<td>Qv</td>
<td>2.11E+05 J/mol</td>
<td></td>
<td>2.11E+11 J/mol</td>
<td></td>
</tr>
<tr>
<td>Qb</td>
<td>1.04E+05 J/mol</td>
<td></td>
<td>1.04E+11 J/mol</td>
<td></td>
</tr>
<tr>
<td>grain width d0</td>
<td>5.00E-04 m</td>
<td></td>
<td>2.50E-01 mm</td>
<td></td>
</tr>
<tr>
<td>Youngs Modulus (E)</td>
<td>1.24E+11 N/m²</td>
<td></td>
<td>1.24E+05 N/mm²</td>
<td></td>
</tr>
<tr>
<td>Poissons ratio (v)</td>
<td>3.50E-01</td>
<td></td>
<td>3.50E-01</td>
<td></td>
</tr>
<tr>
<td>Shear modulus (G)</td>
<td>4.59E+10 Pa</td>
<td></td>
<td>4.59E+04 N/mm²</td>
<td></td>
</tr>
</tbody>
</table>

#### Calculated Parameters

- **Diffusion coefficient (Db)**
  
  \[ Db = Db0 \exp(-Qb/RT) \]

  \[ Db = 4.98E-11 \text{ m}^2/\text{s} \]

- **GB Mobility coefficient (Mgb)**
  
  \[ Mgb = Db \times \delta_b \times \Omega / (kT) \]

  \[ Mgb = 2.08E-29 \text{ m}^4/\text{s/kg} \]

- **Lattice diffusion coeff. (Dv)**
  
  \[ Dv = Dv0 \exp(-Qv/(R_gT)) \]

  \[ Dv = 1.309E-15 \text{ m}^2/\text{s} \]
Appendix D - Derivations for 1 degree of freedom model.

Initial system.

Using Figure 33 the analytical 1 degree of freedom model can be derived. In this model we assume the only variable in the system is the radius of the cavity, we also derive the expressions for the whole system as opposed to only half. The dihedral angle is assumed to remain constant. The variational principle is used in this model as follows:

\[ \Pi = dE \frac{dt}{dt} + 2 \left( \frac{1}{2M_s} \int J_s^2 d\Gamma_s \right) + \frac{1}{2M_{gb}} \int J_{gb}^2 d\Gamma_{gb} \]  
\[(D-1)\]

We know that:

\[ J_s = A.s \]  
\[(D-2)\]

\[ S_{total} = \left( \frac{R\Psi}{2} \right) \]

Where: \( A \) - Constant
\( s \) - surface length

And when:

\( s = S_{total} \) then \( 2.J_s = -J_{gb} \)

Therefore:

\[ 2.J_s = -J_{gb} = V_{gb}I_{gb} = AR\Psi \]
\[ A = \frac{V_{gb}I_{gb}}{R\Psi} \]  
\[(D-3)\]

Inserting (D-3) into (D-2) and changing the variable from \( s \) to \( \theta \) (remembering that \( s = R\theta \)), we arrive at the expression for surface flux in terms of the separation velocity:
Evaluation of surface term.

The surface term can be re-written using (D-4) and changing the variable from \( s \) to \( \theta \).

\[
\frac{1}{2M_s} \int J_s^2 d\Gamma_s = \frac{1}{2M_s} \int_0^\theta \left( \frac{V_{gb} \cdot l_{gb}}{\Psi} \right)^2 \theta^2 d\theta
\]

\[
= \frac{R}{2M_s} \left( \frac{V_{gb} \cdot l_{gb}}{\Psi} \right)^2 \int_0^\theta \theta^2 d\theta
\]

\[
= \frac{V_{gb}^2 \cdot l_{gb}^2 R}{2M_s \Psi^2} \left[ \frac{\Psi^3}{3} - 0 \right]
\]

\[
= \frac{l_{gb}^2 \cdot R \cdot \Psi}{6M_s} \cdot V_{gb}^2
\]

Evaluation of grain boundary term.

The grain boundary term can now be evaluated in the same way:

\[
\frac{1}{2M_{gb}} \int J_{gb}^2 d\Gamma_{gb} = \frac{1}{2M_{gb}} \int V_{gb}^2 \cdot x^2 d\Gamma_{gb}
\]

\[
= \frac{V_{gb}^2}{2M_{gb}} \left[ \frac{x^3 \tau_{gb}}{3} \right]_0
\]

\[
= \frac{V_{gb}^2 \cdot l_{gb}^3}{6M_{gb}}
\]
Evaluation of free energy change rate term.

The final term that needs to be evaluated is the free energy change rate term, this contains the terms due to the applied stress, the change in free surface length and also the extra term which takes into account the opening of the grain boundary.

The expression for \( \frac{dE}{dt} \) is given as:

\[
\frac{dE}{dt} = -\sigma_m \cdot L_0 \cdot V_{gb} + \frac{\Psi}{2} \cdot \frac{dR}{dt} \cdot 2\gamma_s + \gamma_{gb} \sin \left( \frac{\Psi}{2} \right) \cdot \dot{R} + \gamma_s \sin \left( \frac{\Psi}{2} \right) \cdot V_{gb} \tag{D-7}
\]

Re-writing (D-7), we have:

\[
\frac{dE}{dt} = -\sigma_m \cdot L_0 \cdot V_{gb} - \gamma_{gb} \cdot \sin \left( \frac{\Psi}{2} \right) \cdot \dot{R} + \gamma_s \sin \left( \frac{\Psi}{2} \right) \cdot V_{gb} \tag{D-8}
\]

However, it can be seen that in (D-8) above there are terms for both \( \dot{R} \) and \( V_{gb} \). Therefore we need to write one in terms of the other before we can minimise the \( \Pi \) functional. This is shown below.

\[
A_{void} = \frac{R^2}{2} (\Psi - \sin \Psi)
\]

\[
\dot{A}_{void} = \frac{2 \cdot R \cdot \dot{R}}{2} (\Psi - \sin \Psi) = -J_{gb} \gamma_s + V_{gb} \cdot R'
\]

The above term incorporates the effects of the rigid motion of the grains. Where:

\( A_{void} = \text{Area of cavity} \)

\( R' = R \sin \left( \frac{\Psi}{2} \right) \)

Then:

\[
R \cdot \dot{R} (\Psi - \sin \Psi) = +V_{gb} \cdot l_{gb} + V_{gb} \cdot R'
\]

\[
R \cdot \dot{R} (\Psi - \sin \Psi) = V_{gb} \left( R' + l_{gb} \right)
\]
\[ V_{\phi b} = \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} \]  

\( \text{(D-9)} \)

We now have \( V_{\phi b} \) in terms of \( \dot{R} \), this can be used to evaluate the \( \Pi \) functional.

**Evaluation of \( \Pi \) functional.**

The functional \( \Pi \) can now be evaluated by inserting (D-5), (D-6), (D-8) & (D-9) into (D-1):

\[
\Pi = \frac{R^2 \dot{R}^2 (\Psi - \sin \Psi)^2 l^2_{gb} \cdot R \cdot \dot{R}}{(R' + l_{\phi b})^2 \cdot 6 M_x} + \frac{R^2 \dot{R}^2 (\Psi - \sin \Psi)^2 l^3_{gb}}{(R' + l_{\phi b})^2 \cdot 6 M_{gb}} + \gamma_s \Psi \dot{R} + \\
\gamma_s \sin\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} - \gamma_{gb} \sin\left(\frac{\Psi}{2}\right) \cdot \dot{R} - \sigma_x L_0 R (\Psi - \sin \Psi) \\
\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} \\
+ \gamma_s \sin\left(\frac{\Psi}{2}\right) \cdot (\Psi - \sin \Psi) R \\
\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} - \gamma_{gb} \sin\left(\frac{\Psi}{2}\right) - \sigma_x L_0 R (\Psi - \sin \Psi) \\
\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} = 0
\]

Now, using the minimisation:

\[
\frac{\partial \Pi}{\partial \dot{R}} = 0 \quad \text{(D-11)}
\]

We arrive at the following expression for the rate of change of radius:

\[
\frac{\partial \Pi}{\partial \dot{R}} = \frac{R^3 \Psi (\Psi - \sin \Psi)^2 l^2_{gb} \cdot \dot{R}}{3 (R' + l_{\phi b})^2 M_x} + \frac{R^3 (\Psi - \sin \Psi)^2 l^3_{gb} \cdot \dot{R}}{3 (R' + l_{\phi b})^2 M_{gb}} + \gamma_s \Psi + \\
\gamma_s \sin\left(\frac{\Psi}{2}\right) \cdot (\Psi - \sin \Psi) R \\
\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} - \gamma_{gb} \sin\left(\frac{\Psi}{2}\right) - \sigma_x L_0 R (\Psi - \sin \Psi) \\
\left(\frac{\Psi}{2}\right) \cdot \frac{R \cdot \dot{R} (\Psi - \sin \Psi)}{(R' + l_{\phi b})} = 0
\]
\[ \dot{R} = \frac{R^3 \Psi (\Psi - \sin \Psi)^2 l_{gh}^2}{3 (R' + l_{gh})^2 M_s} + \frac{R^2 (\Psi - \sin \Psi)^2 l_{gh}^3}{3 (R' + l_{gh})^2 M_{gh}} = \sigma \alpha \frac{L_0 (\Psi - \sin \Psi)}{(R' + l_{gh})} + \gamma_{gh} \sin \left( \frac{\Psi}{2} \right) \]

\[ \gamma_s \sin \left( \frac{\Psi}{2} \right) (\Psi - \sin \Psi) R \]

\[ -\gamma_s \frac{\sin \left( \frac{\Psi}{2} \right) (\Psi - \sin \Psi) R}{(R' + l_{gh})} \]

\[ \sigma \alpha \frac{R (\Psi_e - \sin \Psi_e)}{L_0} + \gamma_{gh} \sin \left( \frac{\Psi_e}{2} \right) (\Psi_e - \sin \Psi_e) \frac{R}{L_0} \]

\[ \dot{R} = \left( \frac{R^2 (\Psi_e - \sin \Psi_e)^2}{3 I_0^2} \left( \frac{l_{gh}^3}{M_{gh}} + \frac{\Psi_e R l_{gh}^2}{M_{gh}} \right) \right) \]

(D-12)

Where \( l = L_0 - R \sin \Psi_e / 2 \). This gives the final expression for the rate of change of radius for this 1 degree of freedom model. The same method is now used to calculate the new value of radius as that used in the 2 degree of freedom model.
Appendix E – Simplified finite element model derivation.

List of Variables used in Multi-Degree of Freedom Model.

Table E-1 shows the functions that were used in the derivation of the model and also in the computer program. The reason for their use was to aid the derivation process and prevent the possibility of an error occurring during the writing out of the expressions.

Table E-1. Functions defined in computer program.

<table>
<thead>
<tr>
<th>Function</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>$= 0$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$= 0$</td>
</tr>
<tr>
<td>$A_3$</td>
<td>$= \frac{\gamma_c}{\sin \frac{\Psi}{2}} - \frac{\gamma_{ph}}{2 \tan \frac{\Psi}{2}}$</td>
</tr>
<tr>
<td>$A_4$</td>
<td>$= \frac{\Psi}{2} \cos \frac{\Psi}{2} - \sin \frac{\Psi}{2}$</td>
</tr>
<tr>
<td>$A_5$</td>
<td>$= \frac{\Psi}{2} \sin \frac{\Psi}{2} + \cos \frac{\Psi}{2}$</td>
</tr>
<tr>
<td>$A_6$</td>
<td>$= \sin \Psi - \Psi$</td>
</tr>
<tr>
<td>$A_7$</td>
<td>$= -\frac{\Psi}{4} + \frac{\sin \frac{\Psi}{2} \cos \frac{\Psi}{2}}{2}$</td>
</tr>
<tr>
<td>$A_8$</td>
<td>$= -\frac{\Psi}{4} - \frac{\sin \frac{\Psi}{2} \cos \frac{\Psi}{2}}{2}$</td>
</tr>
<tr>
<td>$A_9$</td>
<td>$= 1 - \cos \Psi$</td>
</tr>
<tr>
<td>$A_{10}$</td>
<td>$= \Psi - \sin \Psi$</td>
</tr>
<tr>
<td>$A_{11}$</td>
<td>$= \left(\frac{L_1}{2} - x_g + x_e - x_-\right)$</td>
</tr>
<tr>
<td>$A_{12}$</td>
<td>$= \left(\sin \frac{\Psi}{2}\right)^2$</td>
</tr>
<tr>
<td>$A_{13}$</td>
<td>$= x_c + R \sin \frac{\Psi}{2} - x_g$</td>
</tr>
<tr>
<td>$A_{14}$</td>
<td>$= \left(x_e^2 + x_g^2 + x_{e}^2 + 2x_e x_+ - 2x_e x_g - 2x_+ x_g\right)^{\frac{3}{2}}$</td>
</tr>
<tr>
<td>$A_{15}$</td>
<td>$= -\frac{\Psi}{2} \cos \left(\frac{\Psi}{2}\right) + \sin \left(\frac{\Psi}{2}\right)$</td>
</tr>
<tr>
<td>$A_{16}$</td>
<td>$= -\frac{\Psi}{2} \cos \left(\frac{\Psi}{2}\right) + \sin \left(\frac{\Psi}{2}\right)$</td>
</tr>
<tr>
<td>$A_{17}$</td>
<td>$= \left(x_e - x_+ + x_+ - x_g + \frac{L_2}{3}\right)$</td>
</tr>
<tr>
<td>$A_{18}$</td>
<td>$= \left(x_g - x_e - x_+ + \frac{L_2}{5}\right)$</td>
</tr>
<tr>
<td>$A_{19}$</td>
<td>$= -x_e - x_+ + x_g + \frac{L_2}{3}$</td>
</tr>
<tr>
<td>$A_{20}$</td>
<td>$= x_e + x_+ - x_g - \frac{3L_2}{8}$</td>
</tr>
<tr>
<td>$A_{21}$</td>
<td>$= -x_g + x_e - x_-$</td>
</tr>
<tr>
<td>$A_{22}$</td>
<td>$= \left(x_g^2 - 2x_g x_e + x_e^2 + x_{e}^2 - 2x_e x_+ + x_+^2\right)$</td>
</tr>
<tr>
<td>$A_{23}$</td>
<td>$= \left(2x_e - 2x_g - 2x_+ + \frac{3L_1}{4}\right)$</td>
</tr>
<tr>
<td>$A_{24}$</td>
<td>$= \left(x_g - x_e + x_+ - \frac{L_1}{3}\right)$</td>
</tr>
<tr>
<td>$A_{25}$</td>
<td>$= x_c - x_g - R \sin \frac{\Psi}{2}$</td>
</tr>
<tr>
<td>$A_{31}$</td>
<td>$= \left(x_e L_2 x_e + x_g L_2 - \frac{L_2^2}{2} - L_1 A_{11}\right)$</td>
</tr>
</tbody>
</table>
Table E-2 shows the combined variable expressions that were used in the derivation and computer program. These are a progression from the functions given in the previous table.

**Table E-2. Combined variable expressions.**

<table>
<thead>
<tr>
<th>Expression 1</th>
<th>Expression 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_{13} = \frac{\Psi}{4} - \frac{\sin \frac{\Psi}{2} \cos \frac{\Psi}{2}}{2} )</td>
<td>( A_{32} = 2 \left( 1 - \cos \frac{\Psi}{2} \right) )</td>
</tr>
<tr>
<td>( A_{14} = \frac{\Psi}{4} + \frac{\sin \frac{\Psi}{2} \cos \frac{\Psi}{2}}{2} )</td>
<td>( A_{33} = \frac{R \Psi^2}{4} )</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
B_1 &= R(A_{10} + A_{16}) \\
B_2 &= 0 \\
B_3 &= L_1^2 \left( \frac{L_1^2}{20} + \frac{A_{11}L_1}{4} + \frac{A_{29}L_1}{3} \right) \\
B_4 &= \frac{A_{23}L_1^3}{3} \\
B_5 &= \frac{A_{24}L_1^2}{2} \\
B_6 &= \frac{A_{17} + A_{13}}{A_9} \\
B_7 &= \frac{A_{19}L_2^2}{3} \\
B_8 &= \frac{2A_{20}L_2^3}{3} \\
B_9 &= L_2 - L_1 \\
B_{10} &= \frac{-A_{12} \sin \frac{\Psi}{2}}{A_9} \\
B_{11} &= \left( B_{12}B_{15} - R \cos \frac{\Psi}{2} \right) \\
B_{12} &= \frac{\sin \frac{\Psi}{2}}{A_9} \\
B_{13} &= 2RA_{16} - \frac{A_{12}B_1}{4} \\
B_{14} &= A_{32}R \cos \frac{\Psi}{2} \\
B_{15} &= \left( RA_{4} - \frac{B_1}{2} \right) \\
B_{16} &= \frac{B_9}{2} + L_1 \\
B_{17} &= \frac{A_{31}}{2} + L_1A_{11} \\
B_{18} &= \frac{2}{A_9R^2} \\
B_{19} &= 2\gamma_sR - R\gamma_{st}\cos \left( \frac{\Psi}{2} \right) \\
B_{20} &= 0 \\
B_{21} &= 0 \\
B_{22} &= 0 \\
B_{23} &= 0 \\
B_{24} &= 0 \\
B_{25} &= 2RA_{4} - \frac{A_{32}B_1}{4} \\
\end{align*}
\]
Free energy change rate derivation.

Taking the time derivative of (5.2-1), the free energy change rate can be derived as:

$$
\dot{G} = \frac{d}{dt} \left( 2\Psi R y_s + \left( x^+ + x^- - 2R \sin \frac{\Psi}{2} \right) y_{gh} - \sigma_{\infty} (x^+ + x^-) B - M\theta \right) + \dot{G}_{\text{junction}}
$$

where $\dot{G}_{\text{junction}}$ is the contribution from grain boundary opening given by (4.3-21).

However there is an extra term $(M\theta)$, to take account of the rotation of the grains. Thus we finally arrive at the expression for free energy change rate:

$$
\dot{G} = \dot{G} \left( 2\Psi R y_s - 2\gamma_{gh} \sin \frac{\Psi}{2} + B_{15} B_{18} B_{19} \right) + J_0^2 \left( \frac{-B_{18} B_{19}}{2} \right) + \\
+ J_0 \left( \frac{-B_{18} B_{19}}{2} \right) + \omega \left( (B_{17} B_{18} B_{19} + A_3 (A_{15} + A_{23})) - M \right) + \\
+ V \left( B_{16} B_{18} B_{19} + 2A_3 - \sigma_{\infty} B_{20} \right)
$$

Surface flux term derivation.

The surface flux is given by (5.2-17) as:

$$
J_s = R R \left( \theta - \sin \theta \cos \frac{\Psi}{2} \right) - R x_s \left( \cos \theta - \cos \frac{\Psi}{2} \right) + \frac{R R^2}{2} \sin \theta \sin \frac{\Psi}{2} + J_s^0
$$

The surface flux term is then evaluated to give a final expression by (5.2-22). The expression is too long to be quoted explicitly but is given in the collected degrees of freedom section later in the appendix.

$$
2 \int J_s^2 \frac{d\Gamma_s}{2M_s}
$$

Grain boundary flux term derivation.

The grain boundary flux expressions for the left and right hand side are given by Equations (5.2-15) and (5.2-16) respectively as:
Hence the grain boundary flux term for each side can be evaluated using (5.2-23):

$$\int \frac{J_{gb}^2}{2M_{gb}} d\Gamma_{gb}$$

This yields the final expressions for grain boundary flux as:

$$J_{gb_{wo}} = \frac{1}{2M_{gb}} \left[ \omega^2 B_3 + \omega V B_4 + \alpha J_0^1 B_3 + V^2 \frac{L_1^3}{3} - V J_0^1 L_1^2 + (J_0^1)^2 L_1 \right]$$

$$J_{gb_{wq}} = \frac{1}{2M_{gb}} \left[ \omega^2 B_6 + \omega V B_8 + \alpha J_0^2 B_7 + V^2 \frac{L_1^3}{3} - V J_0^2 L_2^2 + (J_0^2)^2 L_2 \right]$$

We now collect the terms for each of the elemental degrees of freedom, the elemental viscosity matrix terms are:

$$A_{RR} = \frac{2}{M_s} \left[ B_{12} (B_{25} + B_{13}) + B_{11} (A_7 + A_{13}) + \frac{R^2 \Psi^3}{12} \right]$$

$$A_{PV} = \frac{1}{M_s} \left[ 2B_{12}^2 B_{16} (A_{13} - A_7) + \frac{\Psi B_2^2}{8} \right] + \frac{1}{3M_{gb}} (L_1^2 + L_2^2)$$

$$A_{wq} = \frac{1}{M_s} \left[ 2B_{12}^2 B_{16} (A_{13} - A_7) + \frac{\Psi A_{s1}}{8} \right] + \frac{1}{M_{gb}} [A_3 + A_6]$$

$$A_{\omega \omega} = \frac{1}{M_s} \left[ \frac{B_{12}^2}{2} (A_{13} - A_7) + \frac{\Psi}{8} \right] + \frac{L_1}{M_{gb}}$$

$$A_{\omega \omega} = \frac{1}{M_s} \left[ \frac{B_{12}^2}{2} (A_{13} - A_7) + \frac{\Psi}{8} \right] + \frac{L_2}{M_{gb}}$$

$$A_{\omega \omega} = \frac{2}{M_s} \left[ R^2 (-A_8 + A_{14} + 2 \sin \Psi) + \Psi R^2 \cos^2 \frac{\Psi}{2} \right]$$
APPENDIX E – SIMPLIFIED FINITE ELEMENT MODEL DERIVATION.

\[ A_{x,R} = A_{x_0} = \frac{1}{M_s} \left[ B_1 R \sin \frac{\Psi}{2} \right] \]

\[ A_{\varphi_0} = A_{\varphi_0'} = \frac{1}{M_s} \left[ 2B_1^2 B_{16}(A_7 + A_{13}) + \frac{\Psi A_{31} B_9}{8} \right] + \frac{(B_4 + B_8)}{2M_{gb}} \]

\[ A_{Rd} = A_{Rd'} = \frac{1}{M_s} \left[ B_{11} B_{12} (A_7 - A_{13}) + \frac{B_{12}}{2} (B_{25} - B_{13}) \right] \]

\[ A_{R} = A_{\varphi R} = \frac{1}{M_s} \left[ 2B_{11} B_{12} B_{17} (-A_7 + A_{13}) + B_{12} B_{17} (B_{13} - B_{25}) \right] \]

\[ A_{x'v} = A_{x_0'} = \frac{1}{M_s} \left[ -B_9 R \sin \frac{\Psi}{2} + \frac{B_9 R \Psi \cos \frac{\Psi}{2}}{2} \right] \]

\[ A_{\varphi d} = A_{\varphi d'} = \frac{1}{M_s} \left[ \frac{B_{12}^2}{2} (-A_7 + A_{13}) - \frac{\Psi}{8} \right] \]

\[ A_{\varphi v} = A_{\varphi d} = \frac{1}{M_s} \left[ B_{12}^2 B_{16} (A_7 - A_{13}) + \frac{\Psi B_9}{8} \right] - \frac{E_s}{2M_{gb}} \]

\[ A_{x_0} = A_{x_0'} = \frac{1}{M_s} \left[ B_{12}^2 B_{17} (A_7 - A_{13}) + \frac{\Psi A_{31}}{8} \right] + \frac{B_7}{2M_{gb}} \]

\[ A_{xv} = A_{x_0} = \frac{1}{M_s} \left[ 2B_{11} B_{12} B_{16} (-A_7 + A_{13}) + B_{12} B_{16} (B_{13} - B_{25}) \right] \]

\[ A_{x_0 v} = A_{x_0 v'} = \frac{1}{M_s} \left[ -A_{31} R \sin \frac{\Psi}{2} + \frac{A_{31} R \Psi \cos \frac{\Psi}{2}}{2} \right] \]

\[ A_{\varphi_0 d} = A_{\varphi_0 d'} = \frac{1}{M_s} \left[ B_{11} B_{12} (A_7 - A_{13}) + \frac{B_{12}}{2} (B_{25} - B_{13}) \right] \]

\[ A_{x_0 u} = A_{x_0 u'} = \frac{1}{M_s} \left[ B_{12}^2 B_{17} (A_7 - A_{13}) + \frac{\Psi A_{31}}{8} \right] - \frac{B_7}{2M_{gb}} \]
APPENDIX E – SIMPLIFIED FINITE ELEMENT MODEL DERIVATION.

\[ A_{x'x} = A_{xx} = \frac{1}{M_x} \left[ R \sin \frac{\Psi}{2} + \frac{R \Psi \cos \frac{\Psi}{2}}{2} \right] \]

\[ A_{x'y'} = A_{yy} = \frac{1}{M_y} \left[ -R \sin \frac{\Psi}{2} + \frac{R \Psi \cos \frac{\Psi}{2}}{2} \right] \]

\[ A_{x'v} = A_{v'x} = \frac{1}{M_s} \left[ B_{12} B_{16} (A_7 - A_5) + \frac{W B_0}{8} \right] - \frac{L}{2M_g} \]

and, the elemental force vector terms are given by:

\[ B_w = B_{17} B_{18} B_{19} + A_3 A_{35} + A_5 A_{15} \]

\[ B_R = 2 \gamma \Psi - 2 \gamma_b \sin \Psi / 2 + B_{13} B_{18} B_{19} \]

\[ B_v = B_{16} B_{18} B_{19} + 2 A_5 \]

\[ B_{h'} = -\frac{B_{18} B_{19}}{2} \]

\[ B_{j'} = -\frac{B_{18} B_{19}}{2} \]

\[ B_{\phi} = 0 \]

We now assemble the elemental matrices using:

\[ \Pi = \sum_{e=1}^{n} \frac{1}{2} \left[ V \omega \right] J_0 J_0^2 \dot{R} \dot{x}_c \left[ V \omega \right] \left[ B_v \right] \]

\[ \left[ A_{v'v} A_{v'\omega} A_{v'J_0} A_{v'J_1} A_{v'J_2} A_{v'R} A_{v'x_c} \right] \left[ V \omega \right] J_0 J_0^2 \dot{R} \dot{x}_c \left[ B_v \right] \left[ B_v \right] \left[ V \omega \right] \]

where \( e \) denotes the number of the element and \( n \) denote the total number of elements in the system. Using appropriate minimizations (\( \partial \Pi = 0 \)) leads to:

\[ [A][X] = [B] \]

where \([A]\) is the global viscosity matrix, \([X]\) holds the global degrees of freedom and \([B]\) is the global force vector. This is shown by (5.2-28).
Mass conservation at the cavity tips.

Mass conservation has to be satisfied at the two cavity tips and the following expression is used to equate the surface and grain boundary flux expressions:

\[ 2J_{x_{l_h}} = -J_{gb_{x_{l_h}}} \]  \hspace{1cm} (E-2)

Starting from the expression for surface flux given by (5.2-17);

\[ J_x = R\hat{R} \left( \theta - \sin \theta \cos \frac{\Psi}{2} - R\hat{x}_c \left( \cos \theta - \cos \frac{\Psi}{2} \right) + \frac{\Psi R^2}{2} \sin \theta \sin \frac{\Psi}{2} + J_s^0 \right) \]

we set \( \theta = -\Psi/2 \) for the left-hand cavity tip and \( \theta = \Psi/2 \) for the right. From this we arrive at two expressions for surface flux, one for the left-hand cavity tip and one for the right. These are shown below:

\[ J_{x_{l_h_{left}}} = \frac{R\hat{R}A_{l_h}}{2} + \frac{\Psi R^2 A_{l_h}}{4} + J_s^0 \]  \hspace{1cm} (E-3)

\[ J_{x_{l_h_{right}}} = \frac{R\hat{R}A_{l_h}}{2} - \frac{\Psi R^2 A_{l_h}}{4} + J_s^0 \]  \hspace{1cm} (E-4)

If we consider the right-hand cavity tip first: at the tip \( L_2 = x^+ - R \sin(\Psi/2) \) and the grain boundary flux becomes:

\[ J_{gb_{x_{r_h}}}^2 = -VL_2 - axcL_2 - ax^+L_2 + axcL_2 + \frac{\omega L_2}{2} + J_s^0 \]  \hspace{1cm} (E-5)

Now, inserting (E-4) and (E-5) into (E-2), we arrive at an expression for surface flux, \( J_s^0 \):

\[ J_s^0 = \frac{1}{4} \left[ VB_3 + \omega A_{c1} + J_s^0 - J_{gb_{x_{r_h}}}^2 - R B_1 \right] \]  \hspace{1cm} (E-6)

If we now consider the left-hand cavity tip: at the tip \( L_1 = x^- - R \sin(\Psi/2) \) and the grain boundary flux expression becomes:

\[ J_{gb_{x_{l_h}}}^1 = -VL_1 - \frac{\omega L_1^2}{2} + axcL_1 - axcL_1 + axcL_1 + J_s^0 \]  \hspace{1cm} (E-7)
Now, inserting (E-3), (E-6) and (E-7) into (E-2), we arrive at an expression for the rate of change of dihedral angle, $\Psi$:

$$\Psi = \frac{2}{A_2 R^2} \left[ \dot{R} \left( A_5 R - \frac{B_1}{2} \right) + V \left( \frac{B_2}{2} + L_1 \right) + \omega \left( \frac{A_{31}}{2} + L_1 A_{11} \right) - \frac{J_0}{2} - \frac{J_0^2}{2} \right]$$

Using the expression defined at the beginning of this appendix, the above expression can be re-written as:

$$\Psi = \dot{R} B_{15} B_{18} + V B_{16} B_{18} + \omega B_{17} B_{18} + J_0 \frac{B_{18}}{2} + J_0^2 \frac{B_{18}}{2} \quad (E-8)$$
Appendix F – Empirical solution parameters.

Miscellaneous computer model information.

This appendix outlines the various processes and functions that have been included in the computer model to allow it to function correctly. Most of the decisions taken for critical sizes or lengths are arbitrary ones and cannot be fully justified. However, they were chosen using a logical decision making process and have resulted in the program functioning correctly. They are in no particular order and are only explained in brief.

1. Use of index array to keep track of changes.

The method used to store the data on the cavity ‘elements’ i.e. positions, sizes, mobilities etc is not a straightforward one. This is due to the nucleation of new cavities and to avoid the need to re-order the entire array when a new cavity is nucleated. If a standard method were used the arrays would have to be continually changed to make room for the nucleated cavities. For example, the system could have 200 elements, but the new cavity could be at the beginning of the grain boundary, therefore all 200 entries in the array would have to be moved along one to make space at the start of the array for the nucleated cavity. To avoid this an ‘INDEX’ array was used that keeps track of the physical position of the elements on the grain boundary and the position the data is stored at in the arrays. The ‘INDEX’ array is a vector with the value of the row corresponding to the position in the other arrays holding the data for the element.

| Index[0] = 0 | Index[0] = 0 |
| Index[1] = 1 | Index[1] = 3 (new cavity) |
| After nucleation | Index[3] = 2 |

The above example shows how the index array works when a cavity in nucleated. The ‘INDEX’ array is re-ordered to make space for the new cavity, however the value held in the array points to the last entry in the array holding the actual cavity data. In this case the new cavity radius would be located using the following method:
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Radii[index[1]] = Radii[3]  \[Which is the last entry in the Radii array.\]

The index array is also used when cavities coalesce. This is to prevent the arrays holding the cavity data from being re-ordered to remove one of the elements, as they have merged into one. When two cavities coalesce the first element is always retained in the arrays and the second element is discarded. The new element being resized and holding the data for the coalesced cavity. The second element is no longer required and to prevent the program from ‘seeing’ it, the value in the ‘INDEX’ array is made negative. This is shown below:

<table>
<thead>
<tr>
<th>Index[0]</th>
<th>Index[1]</th>
<th>Index[2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

\(\Rightarrow\) \(\Rightarrow\) \(-2\)  \[coalesced cavity\]  \[discarded cavity\]

2. Re-starting the model after a crash or stoppage.
The program has the ability to be re-started from the last position a data file was written. This is to allow the simulation to continue after it had been stopped for any reason, instead of having to start from the beginning again. The program writes a file called ‘data.out’ every time the results file is written. This file contains all the current values of the system parameters and current time and can be used as a restart file.

3. Preventing cavities being updated when they reach the end of the system.
The ends of the system are normally sealed when running simulations, and as such require some special attention when cavities approach them. If the cavities nearest the ends were allowed to continue growing once they reached the ends of the system it would cause the program to become unstable and produce erroneous results. Therefore, when cavities grow to such an extent that they reach the sealed ends of the system they are no longer updated. The cavities remain part of the model and the rate equations are solved each timestep but the values are not updated.

The reason for the use of ‘buffer zones’ is the empirical based nucleation law that is used in this model. The nucleation law is based on observed nucleation. If the nucleated
cavities were placed too close to existing cavities they would coalesce instantly. These cavities would not be observed as being nucleated and would be inconsistent with the nucleation law being used. The program uses ‘buffer zones’ around the cavity, these are designed to prevent the nucleated cavities from getting too close to the existing cavities and causing a negative length to occur or coalescing instantly. Negative lengths occur when the nucleated cavity overruns into the existing cavity and there is not enough space to place a node between the two elements. The size of the ‘buffer zone’ is arbitrary but in this model is has been defined as the critical cavity half-length. Therefore, if a new cavity is placed on the edge of the buffer zone it will not reach the next element and cause a problem.

5. Selection of valid grain boundary for nucleation.
The method used for selecting which segments of grain boundary are suitable for nucleation of cavities is based on a single length; the critical segment length (csl). The program scans through the system of cavities and calculates the length of the grain boundary segments in each element. If the segment is longer than the csl then it is stored in an array along with all information relevant to the segment. If the segment is shorter than the csl it is ignored. The remaining grain boundary is then summed and the total found. This is the total length of ‘good’ grain boundary, i.e. grain boundary that has no cavities on it. The random number generated is then applied to this total and a position is found on the good grain boundary for the nucleation to take place. The segment corresponding to this position is identified and the position is mapped back on to the actual system to take account of the cavities and ‘buffer zones’. This avoids the problem of the random position falling on an existing cavity or node. The program then proceeds to nucleate the cavity at this point.