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Meso–Scale Modelling of Deformation, Damage and Failure in Dual Phase Steels

By

Iman Sari Sarraf

A Dissertation
Submitted to the Faculty of Graduate Studies through the Department of Mechanical, Automotive & Materials Engineering in Partial Fulfilment of the Requirements for the Degree of Doctor of Philosophy at the University of Windsor

Windsor, Ontario, Canada

2017

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Declaration of Co-Authorship and Previous Publication

I Co-Authorship Declaration

I hereby declare that this dissertation incorporates material that is the result of joint research undertaken in collaboration with Dr. Sergey Golovashchenko, Dr. Kevin P. Boyle, Dr. Javad Samei, Dr. Amir Hassannejad, Mr. Arash Jenab, Mr. Dan Mario Vasilescu, Mr. Yang Song, and Mr. Brent McCallum under the supervision of Prof. Daniel E. Green, University of Windsor. In addition, Dr. Javad Samei and Mr. Brent McCallum provided the material characterization of DP600 steel sheets, and Mr. Dan Mario Vasilescu and Mr. Yang Song collaborated in performing rolling with subsequent uniaxial tension tests. In all cases, the key ideas, the primary contributions, simulations and data analysis and interpretations were performed by the author of this dissertation. The contributions of the co-authors were primarily focused on the provision of the study and suggesting possible directions. Results related to this research are reported in Chapters 4 through 7, inclusively.

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Abstract

Advanced high strength steels (AHSS), such as dual phase (DP) and transformation induced plasticity (TRIP) steels, offer high ductility, formability, and strength, as well as high strength-to-weight ratio and improved crash resistance. Dual phase steels belong to a family of high strength grades which consist of martensite, responsible for strengthening, distributed in a ductile ferrite matrix which accommodates the deformation throughout the forming process. It has been shown that the predominant damage mechanism and failure in DP steels depends on the ferrite and martensite grain sizes and their morphology, and can range from a mixture of brittle and ductile rupture to completely ductile rupture in a quasi-static uniaxial tension test. In this study, a hybrid finite element cellular automata model, initially proposed by Anton Shterenlikht (2003), was developed to evaluate the forming behaviour and predict the onset of instability and damage evolution in a dual phase steel. In this model, the finite element constitutive model is used to represent macro-level strain gradients and a damage variable, and two different cell arrays are designed to represent the ductile and brittle fracture modes in meso-scale. In the FE part of the model, a modified Rousselier ductile damage model is developed to account for nucleation, growth and coalescence of voids. Also, several rate-dependent hardening models were developed and evaluated to describe the work hardening flow curve of DP600. Based on statistical analysis and simulation results, a modified Johnson-Cook (JC) model and a multiplicative combination of the Voce-modified JC functions were found to be the most accurate hardening models.

The developed models were then implemented in a user-defined material subroutine (VUMAT) for ABAQUS/Explicit finite element simulation software to simulate uniaxial tension tests at strain rates ranging from 0.001s\(^{-1}\) to 1000s\(^{-1}\), Marciniak tests, and
electrohydraulic free-forming (EHFF). The modified Rousselier model could successfully predict the dynamic behaviour, the onset of instability and damage progress in DP600 tensile test specimens. Also, the forming limit curve (FLC) as well as the final damage geometry in DP600 Marciniak specimens was successfully predicted and compared with experiments. A hybrid FE+CA model was utilized to predict the major fracture mode of DP600 and DP780 sheet specimens under different deformation conditions. This hybrid model is able to predict quasi-cleavage fracture in ultra-fine and coarse-grained DP600 and DP780 at low and high strain rates. The numerical results showed the capabilities of the proposed model to predict that higher martensite volume fraction, greater ferrite grain sizes and higher strain rates promote the brittle fracture mechanism whereas finer grain sizes and higher temperature alter the dominant fracture mechanism to ductile mode.
Dedication

To my beloved wife, Niloufar

and

my parents
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First and foremost, I would like to express my deepest gratitude to my experienced advisor, Dr. Daniel E. Green for his relentless guidance, care, patience, and for providing me with excellent help and support for conducting research. His positive outlook and encouragements in my research inspired me and gave me confidence and motivation to pursue my research interest. Thank you for believing in me and giving me a unique opportunity to work on such an important and interesting topic. He is, by far, one of the best supervisors one can imagine.

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I owe a great debt of gratitude to my parents who raised me up “to more than I can be”. Their constant, continuous and infinite love, sacrifices, encouragements and supports helped me to move forward in my life. I would like to thank my sister, Naghme, who is the main inspiration of my life, whose limitless kindness and support helped me a lot through different stages of my life. Finally, I would like to say billions of thanks to my beloved wife, Niloufar, for her infinite and unconditional support, love, and encouragement. Without her persistent help, this work would not have been possible. Her beautiful smile, even at tough times, kept me alive.
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Nomenclature

Chapter 4

\( \beta \)  scalar damage variable
\( \beta_c \)  critical damage value at failure
\( \dot{\varepsilon}_0 \)  reference strain rate
\( \dot{\varepsilon}_p \)  equivalent plastic strain rate
\( \lambda \)  plastic multiplier in the normality rule
\( \sigma_m \)  hydrostatic stress
\( \sigma_s \)  saturation stress
\( \sigma_{eq} \)  von Mises equivalent stress
\( \varepsilon_p \)  equivalent plastic strain
\( B \)  conjugate force of damage parameter
\( C_{1...n} \)  material constants or predictors in the hardening equations
\( D , \sigma_I \)  adjustable Rousselier damage model parameters
\( D_0^p \)  upper bound strain rate
\( E \)  Young’s modulus
\( f \)  current void volume fraction
\( f_0 \)  initial void volume fraction
\( f_c \)  critical void volume fraction at failure
\( H \)  hardening curve of the material

Chapter 5

\( \alpha_t , \beta_t \)  Thomason coalescence model coefficients
\( \beta \)  scalar damage variable
\( \chi \)  void space Ratio
\( \delta \)  multiplicative void growth acceleration factor
\( \dot{\varepsilon} \)  strain rate
\( \varepsilon_0 \) reference strain rate
\( \eta \) function of void distribution
\( \gamma \) cell geometry related coefficient
\( \lambda \) plastic multiplier in the normality rule
\( \sigma_I \) maximum principal stress
\( \sigma_m \) hydrostatic stress
\( \sigma_{eq} \) equivalent stress
\( \varepsilon_c \) critical strain at the onset of coalescence
\( \varepsilon_f \) fracture strain
\( \varepsilon_N \) mean strain at void nucleation
\( \varepsilon_p \) equivalent plastic strain
\( \varepsilon_{I,II,III} \) principal plastic strains
\( \vartheta \) current void distribution
\( \vartheta_0 \) initial void distribution
\( B \) conjugate force of damage parameter
\( C_{1...n} \) fitting parameters of hardening functions
\( D, \sigma_1 \) adjustable Rousselier damage model parameters
\( D_0^p \) arbitrary upper bound strain-rate
\( f \) current void volume fraction
\( f^* \) effective void volume fraction
\( f_0 \) initial void volume fraction
\( f_c \) critical void volume fraction at the onset of coalescence
\( f_f \) void volume fraction at failure
\( f_N \) volume fraction of void nucleating particles
\( f_u^* \) final effective void volume fraction at final damage
\( H_0 \) initial height of the unit cell
\( n \) strain hardening exponent
$R$ hardening curve of material
$r$ radius of the void
$R_0$ initial radius of the unit cell
$S_N$ standard deviation
$W$ void aspect ratio
CN cluster nucleation
SCVN strain controlled void nucleation

**Chapter 6**

\(\alpha_t, \beta_t\) Thomason coalescence model coefficients
\(\beta\) scalar damage variable
\(\beta_f\) critical Rousselier scalar damage variable at failure
\(\chi\) void space Ratio
\(\dot{\varepsilon}_p\) equivalent plastic strain rate
\(\lambda\) plastic multiplier in the normality rule
\(\Phi_d(f)\) stored damage energy
\(\Phi_e(\varepsilon_e)\) stored elastic energy
\(\Phi_p(\varepsilon_p)\) stored plastic energy
\(\sigma_I\) maximum principal stress
\(\sigma_m\) hydrostatic stress
\(\sigma_{eq}\) equivalent stress
\(\varepsilon_c\) critical plastic strain at failure
\(\varepsilon_e\) elastic strain
\(\varepsilon_N\) mean strain at void nucleation
\(\varepsilon_p\) equivalent plastic strain
\(\varepsilon_{I,II,III}\) principal plastic strains
\(B\) conjugate force of damage parameter
\(C_{1...n}\) fitting parameters of hardening functions
$D$, $\sigma_k$ adjustable Rousselier damage model parameters

- $f$: current void volume fraction
- $f^*$: effective void volume fraction
- $f_0$: initial void volume fraction
- $f_c$: critical void volume fraction at the onset of coalescence
- $f_f$: void volume fraction at failure
- $f_N$: volume fraction of void nucleating particles
- $f_u^*$: final effective void volume fraction at final damage

- $H(\varepsilon_p)$: hardening curve of material
- $n$: strain hardening exponent
- $S_N$: standard deviation
Chapter 1

Introduction

1.1 Dual phase steels

The automotive industry is constantly challenged to decrease fuel consumption, improve safety, reduce weight and enhance the crash response of auto-body structures. Advanced high-strength steels (AHSS) have been developed to fulfil these requirements and be used for automotive structural components in order to improve manufacturability, durability and crash-worthiness without corresponding weight increases. Among all AHSS categories, dual phase (DP)-type steels and transformation-induced plasticity (TRIP)-type steels are the most widely-used. The term dual-phase was first coined by Hayami and Furukawa as a family of high-strength cold-rolled steels. Dual phase steels are low carbon micro-alloyed steels that usually consist of 70-90 Vol% of ductile ferrite matrix and around 5-30 vol% of dispersed hard martensite. Usually, small amounts of other phases such as bainite, pearlite or retained austenite can possibly be found in the DP steel microstructure and can affect their physical and mechanical properties. This composite microstructure can be achieved through the special heat treatment regime that consists of inter-critical annealing in the $\alpha + \gamma$ with subsequent quenching.
The mechanical and forming properties of DP steels, in terms of high ductility and strength, are the direct result of their composite-like microstructure where the ductile ferrite matrix contributes to good cold formability and the hard martensite operates as the strengthening element. The correct proportion of each of the two phases leads DP steels to exhibit great mechanical characteristics such as continuous yielding, high strain hardening rates at low strain values and large uniform elongation \[7\text{--}11\], which results in their increasing application for auto-body members. The application of various grades of DP steels for different components in a car, such as bumper beam, A-frame reinforcement, roof bow, B-pillar reinforcement, rear side member, front floor cross member and floor side reinforcement is shown in Fig. 1.1.

![Figure 1.1: Application of DP steels in a typical automobile](image)

To evaluate the forming and failure behaviour of DP steels, different tests have been carried out at various strain rates ranging from quasi static conditions (0.001 s\(^{-1}\)) to high strain rates (5000 s\(^{-1}\) using a split Hopkinson bar \[14\text{--}15\]) and strain paths using different deformation processes and test procedures \[16\text{--}17\]. Based on obtained experimental results, different constitutive hardening functions and damage models, either
phenomenological or micro-mechanical models, have been developed and calibrated to be implemented in commercial finite element simulation software such as ABAQUS or LS-Dyna for formability analysis and for crash simulations.

Due to the microstructure of DP steels and the interaction of ferrite and martensite grains during a deformation process, four different mechanisms have been identified for fracture initiation: (a) martensite cracking, (b) decohesion at ferrite-martensite interfaces, (c) decohesion at ferrite-ferrite interfaces, and (d) decohesion at the interface between two adjacent martensite grains [6,18–20]. The main mechanisms of fracture can alter from a fully ductile fracture mode with dimples and voids to a completely brittle fracture mode with well-defined facets and cleavage steps on these facets [21]. Nevertheless, conventional numerical approaches and FE simulation software are not able to distinguish these mechanisms that are directly related to the microstructural properties of DP steels. Accordingly, new approaches or models should be employed to fill this gap and take microstructural properties into account.

1.2 Hybrid finite element cellular automata method

The finite element method (FEM) is one of the most widely-used approaches to predict the stress, strain and temperature distribution, deformation history and damage accumulation under a specific applied force or forming process and evaluate the forming and failure behaviour of materials. The accuracy of a FE simulation of a sheet metal forming process is directly dependent on the constitutive material model which describes the elasto-plastic behaviour with a hardening function, i.e. true stress-strain flow curve, and the contact condition. Therefore, different factors should be evaluated to choose the most accurate and suitable constitutive material model for a FE sheet metal forming analysis. Moreover, since post-uniform deformation commences by the formation of a small diffuse or localized necking, a quantitative prediction of the limiting strain therefore requires assessment of both necking and failure. It is shown that there are two major sources that contribute to localization: (1) the microstructure of the material such as second phase particles, grain morphology
and surface defects \[22-24\] and (2) the constitutive behaviour in terms of hardening, softening and strain-rate sensitivity \[25, 26\].

As described by Shterenlikht \[27\], the main problem in conventional finite element analysis software is that a FE is both a material and a structural unit simultaneously. Therefore, they fail to address the micro-scale microstructural features and properties in evaluating the damage mechanisms in non-homogeneous materials. On the other hand, large numbers of small finite elements are needed to analyse the damage behaviour and fracture propagation under a certain stress state which results in high computational cost. Determining the size of elements, to correctly represent the stress and strain gradients, in the refined meshed region strongly depends on the nature of possible fracture mechanism due to the microstructural features present in a material. This makes determining the size scale of finite elements difficult when simulating the behaviour of multi-phase materials since the finite element mesh in front of a crack tip should be highly refined due to the physical nature of brittle damage mechanism whereas the element size for evaluating the ductile fracture mode is a function of spacing between microvoids or large inclusions which is considerably larger than that required for evaluating brittle fracture. The only solution in a conventional FE simulation is to select a compromise mesh size \[27, 28\]. The main approach for solving these problems is to separate the material and microstructural properties from the mechanical properties and move them to another entity. Accordingly, different numerical models have been established and developed based upon digital material representation to take the microscale features of different materials into account in the simulation of various forming processes \[6, 29-31\].

Although the combination of cellular automata and FE has been used for solidification or recrystallization of materials, Beynon et al. \[32\] and Shterenlikht \[27, 28\] were the first to utilize it for evaluating forming and damage behaviour of steels. In this model, the microstructural properties of the material is moved from the finite elements to an appropriate number of cells in two independent cell arrays, responsible for ductile and brittle fracture mechanisms. Therefore, the FE mesh is employed to represent the macro-level strain and stress tensors and damage variables, and the cellular automata arrays with independent and desired size scales are utilized to
analyse the microstructural response of the material. In this hybrid (concurrent) finite element-cellular automata model, the results of different parallel scales are transferred to each other during each simulation time step. The main advantage of this model is its capabilities to simulate forming and damage behaviour in a multi-scale domain so that complex deformation states and their influences on the fracture initiation and propagation can be assessed [6].

1.3 Objectives of the research

The main objective of this research is to investigate, develop and modify microstructurally based models to predict the onset of strain localization and fracture, and implement the new material model in a user-defined material subroutine for a commercial finite element simulation software. The model developed in this study is a combination of finite element analysis method and cellular automata, and has been implemented in a user material subroutine (VUMAT) that is used in ABAQUS/Explicit FE simulation software. As shown in Fig. 1.2, the principal steps in development of the FE model are to:

- conduct a comprehensive review of various micro-mechanical and phenomenological constitutive damage models, hardening functions to describe the dynamic behaviour of the material, void nucleation functions and void coalescence criteria,
- calculate the coefficients of different strain- or strain rate-dependent hardening functions using an appropriate regression method and advanced optimization techniques, as well as utilizing statistical analysis and other methods to evaluate the goodness of the fit and the ability of each existing model and newly developed function to predict the hardening behaviour of the material,
- investigate the role of the constitutive damage model parameters on the flow curve and calibrate them based on different rate-dependent hardening functions,
• implement complementary functions and criteria, such as void nucleation functions and void coalescence criteria, in the model to develop a complete constitutive damage model,

• evaluate the forming and damage behaviour of DP600 subjected to a wide range of testing and deformation conditions, such as uniaxial tension at different strain rates ranging from 0.001 s\(^{-1}\) to 1000 s\(^{-1}\), Marciniak tests, and electro-hydraulic forming (EHF) of laboratory-scale specimens,

• evaluate the capability and performance of the developed damage model in predicting the onset of necking and fracture in a range of metal forming processes, including electrohydraulic forming.

Figure 1.2: Implementing different functions and criteria in the finite element scale constitutive model

The principal goals of this research for developing a hybrid finite element-cellular automata model are to:

• develop a CA model that can take some of the microstructural features into account to evaluate the dominant fracture mode in dual phase steels,
- identify the role of microstructural features in the damage behaviour of dual phase steels and their contribution to ductile and brittle fracture mechanisms in a wide range of deformation conditions, such as uniaxial tension at different strain rates and electro-hydraulic forming (EHF),

- evaluate the capabilities of the developed hybrid model to perform parametric studies based on process parameters (such as strain, strain rate and temperature) and microstructural properties (such as the grain size, and the amount and distribution of martensite).

1.4 Structure of the dissertation

A brief description of the contents of each chapter is presented in the following:

- **Chapter 2** presents a brief review of physical and mechanical properties of dual phase steels, as well as a review of different phenomenological and micromechanical damage models, void nucleation functions and void coalescence criteria

- **Chapter 3** describes the concept of cellular automata, and explains the formulation of the hybrid FE+CA model

- **Chapter 4** defines the non-linear regression (NLR)+ Markov chain Monte Carlo (MCMC) method to calculate the coefficients of the hardening functions. Moreover, the calibration procedure of the Rousselier damage model and the effect of rate-dependent hardening functions on the tensile flow behaviour of DP600, predicted by the Rousselier model is discussed.

- **Chapter 5** defines the implementation procedure of void nucleation functions and void coalescence criteria, and void growth acceleration function in the Rousselier damage model. The performance of the modified constitutive model in predicting the tensile behaviour of DP600 along different strain rates is discussed.
• **Chapter 6** presents the performance of the modified Rousselier damage model in predicting the quasi-static forming limit curve (FLC) of DP600. In addition, damage evolution and accumulation at different strain paths and final damage geometries are investigated.

• **Chapter 7** presents and discusses the results of the hybrid FE+CA model in terms of ductile and brittle damage evolution and the dominant fracture mechanism for different forming conditions.

• **Chapter 8** presents a summary and conclusions of this research as well as some suggestions for future work.

### 1.5 Bibliography


Chapter 2

Literature review

2.1 Advanced high strength steel

There is an increasing demand in the automotive industry to reduce both vehicle weight and gas emissions, and increase fuel efficiency. Therefore, significant effort and energy have been invested to develop suitable materials which can exhibit excellent performance in terms of combined high ductility and strength [1 2]. Automotive steels can be categorized based upon their metallurgical designation to low strength steels, e.g. interstitial free (IF) and mild steels, conventional HSS (carbon manganese, bake hardenable and high-strength, low-alloy steels), ultra-high strength steels (UHSS) and new advanced high strength steels (AHSS), such as dual phase steels (DP), transformation induced plasticity (TRIP) steels. The latter grade of steels (AHSS) offer high strength-to-weight ratio and improved crash resistance [3]. They are complex and sophisticated materials, carefully designed to have certain multiphase structures and microstructural properties achieved by precisely controlled heating and cooling processes. The AHSS family also includes complex-phase (CP), ferritic-bainitic (FB), martensitic (MS or MART), hot-formed (HF), and twinning-induced plasticity (TWIP). They show an excellent combination of high strength and ductility, and have great potential for reducing car weight and improving crash-worthiness [4 5]. The broad range of the formability of different grades of steel as a function of their tensile strength
is shown in Fig. 2.1.

Figure 2.1: Global diagram of total elongation of AHSS grades in comparison with traditional low-strength and high-strength steels

The main difference between conventional HSS and AHSS relies on their microstructure, where HSS are often single-phase ferritic steels with a potential for some pearlite, but AHSS contain a phase other than ferrite or pearlite, such as martensite, bainite or austenite in adequate quantities to exhibit unique mechanical properties.

### 2.1.1 Dual phase steel

The use of dual phase (DP) steels is rapidly growing in the automotive industry due to their superior performance in terms of combined ductility, work hardening rate, strength-to-weight ratio and crash resistance. Dual phase steels (DP), being low carbon steels, belong to a family of high strength strip grades which consist of hard second phase islands (usually martensite) distributed across a ductile ferritic matrix. Therefore, their microstructure usually consists of 5-30 vol% martensite, responsible for strengthening the material, distributed in a ductile ferrite matrix which accommodates the deformation throughout the forming process. To obtain such microstructure, DP steels are intercritically annealed by holding a strip in the ferrite-austenite region for a period of time, followed by controlled quenching so that austenite transforms to soft ferrite and hard martensite, shown in Fig. 2.2. Martensite carbon content \( C_m \) can be determined via mass balance calculation between the carbon content of
the DP steel ($C_c$), carbon content of ferrite ($C_f$) and martensite volume fraction ($f_m$) as shown in Eq. (2.1)

$$C_m = \frac{C_c - C_f}{1 - f_m} (1 - f_m)$$  \hfill (2.1)

Figure 2.2: Schematic diagram of heat treatment methods to obtain dual phase steels (A: austenite, F: ferrite, M: martensite, $A_{c1}$: austenite formation temperature, and $A_{c3}$: ferrite to austenite transformation completion temperature) [12]

Changing the mentioned thermomechanical process will result in the production of various grades of dual phase steels with different microstructural properties in terms of martensite volume content and morphology, ferrite grain size (as shown in Fig. 2.3, 2.4) and mechanical properties [7, 9, 13]. In addition to ferrite and martensite, a small amount of retained austenite may exist in DP steels which reduces the amount of martensite volume fraction. The effect of ferrite and martensite content and their morphology on the mechanical properties and deformation behaviour of DP steels have been extensively studied by different researchers [14–19]. It is shown that the ferrite is continuous for many DP steel grades up to DP780, however, when the martensite volume fraction exceeds 50%, the ferrite becomes discontinuous and martensite islands tend to form a semi-continuous band at the mid-thickness of the sheet [13, 20]. Different regimes of martensite transformation and adding Mn as an alloying element to the
steel are the main responsible sources of developing such microstructural banding in low-alloy steels \cite{21, 23}. Usually, these microstructural bands are not produced during hot rolling and they can be eliminated by high temperature homogenization before intercritical annealing to redistribute alloying elements \cite{23, 24}. DP steels generally show low yield strength and high ultimate tensile strength, continuous yielding behaviour, high strain hardening rates at low strain values and large uniform elongation \cite{3, 25}.

![Thermomechanical procedures to obtain dual phase steels with (a) coarse, (b) fine and (c) ultra-fine grain size.](image)

**Figure 2.3:** Thermomechanical procedures to obtain dual phase steels with (a) coarse, (b) fine and (c) ultra-fine grain size. \(\text{Ar}_3\): non-equilibrium transformation start temperature, \(\text{P}_f\): pearlite transformation finish temperature, and \(\varepsilon\): logarithmic equivalent plastic strain \cite{7}.

![Microstructure of a dual phase steel with (a) coarse grain (CG), (b) fine grained (FG) and (c) ultrafine grain sizes (UFG) achieved by thermomechanical treatment illustrated in Fig. 2.3 showing ferrite (black) and martensite (grey).](image)

**Figure 2.4:** Microstructure of a dual phase steel with (a) coarse grain (CG), (b) fine grained (FG) and (c) ultrafine grain sizes (UFG) achieved by thermomechanical treatment illustrated in Fig. 2.3 showing ferrite (black) and martensite (grey) \cite{7}.

The application of dual phase steels is rapidly growing in the automotive sheet metal forming industry. Usually, conventional low strain-rate processes such as stamping or bending are used to manufacture automotive-parts, such as A-frame reinforcements,
roof bows, B-pillar reinforcements, rear side members, and front floor cross members \cite{26,27}. However, new high strain-rate forming techniques based on explosive forming (EF) and electro-hydraulic forming (EHF), which can increase metal formability and uniform strain distribution and decrease usual forming defects \cite{28,29}, are generating a great interest in the automotive industry. Experimental research has shown remarkable improvement in the formability of DP500, DP600, DP780 and DP980 steel sheets that were formed using an electrohydraulic deformation process \cite{30,31}. Determination of metal formability as well as the onset of localization, instability and failure have become a great interest, yet challenging subject, in both academia and industry. Since limit strains may be preceded by little diffuse or localized necking, a quantitative prediction of the limiting strain therefore requires precise and comprehensive assessment of both necking and failure \cite{32}. Accordingly, the concept of a forming limit curve (FLC) in principal strain space, initially proposed by Keeler and Backofen \cite{33}, and Goodwin \cite{34}, has been extensively used by both academia and industry to evaluate the quasi-static formability of different dual phase steels \cite{6,35–38}. Moreover, Maris et al. \cite{39} derived the high strain rate FLC of DP600 using electrohydraulic free forming (EHFF). Figure. 2.5 shows two examples of the FLC of DP600 that were obtained based on experimental necked data points.
Figure 2.5: Forming limit diagram (FLD) of DP600 obtained in (a) quasi-static condition (open circles are necked data points, $\eta$ is triaxiality and $\beta$ denotes strain ratio) [38] and at (b) high strain rate subject to EHFF [39].
Three stages are identified in the work hardening process of DP steels \[40, 41\]. In the first stage, ferrite grains are deformed homogeneously in the vicinity of martensite islands which is considered as the initial work hardening stage. The second stage consists of limited deformation of the ferrite in the presence of rigid martensite and the third stage occurs when the dislocation density increases and cell structures form due to high strain levels. It has also been shown that a small amount of martensite plasticity can participate in the deformation process in this stage \[20\].

It has been shown by several researchers that the predominant damage mechanism and failure in DP steels depends on the ferrite and martensite grain sizes and their morphology \[7, 42, 43\], and can change from a mixture of cleavage and dimples to a completely ductile failure mechanism which consists of nucleation, growth and coalescence of voids during the forming process \[7, 43\]. Numerous investigations have provided detailed analyses of the microstructure and failure mechanisms in dual phase steels as a function of deformation process parameters (such as strain, strain rate and temperature) and microstructural properties (such as grain size, martensite content and morphology) \[7, 30, 38, 44–52\]. Different mechanisms and potential sites can be involved in the formation of voids in the diffused necking area, as shown in Fig. 2.6. One of the mechanisms of void formation is nucleation in cracked martensite, particles usually when the DP steel contains coarse martensite particles (Fig. 2.6a); inclusions are also important sites for void nucleation (Fig. 2.6b); the dominant mechanism is, however, decohesion at the ferrite-martensite interface (or at triple junctions) (Fig. 2.6c); and finally, void nucleation and also coalescence can take place by the decohesion between two martensite particles along the grain boundary (Fig. 2.6d).
Figure 2.6: Potential sites for void formation or damage initiation in dual phase steels (DP600), (a) fracture of martensite, (b) decohesion of the interfaces between the martensite particles and the ferrite matrix or at the triple junctions, (c) void initiation between two martensite particles along the grain boundary and (d) voids growth along the ferrite grain boundaries and parallel to the direction of the applied tensile load.

Another important factor which determines the dominant fracture mechanism in DP steels, is the grain size due to the dislocation locking and the formation of Cottrell atmospheres and relaxation of internal stresses. Indeed grain size is known to have an effect on the uniform and total elongation of the material. As it can be seen in Fig. 2.7a, the dominant mechanism of failure in a coarse grained DP steel is brittle fracture, identified by well-defined facets and cleavage steps on these facets although a number of dimples can also been observed. The fracture in a fine-grained steel is a combination of both ductile and brittle fracture, while the ultra-fine grain DP steel shows dimples throughout the specimen which indicates a fully ductile fracture.
Figure 2.7: Fracture surface of tensile specimens indicating an increase in non-uniform deformation with decreasing grain size in (a) coarse-grained (12µm) and (b) fine-grained (3µm) and (c) ultra fine-grained (1.5µm) DP steel[7, 51]

Furthermore, Samei et al. [38] showed that strain path also has significant effect on the damage and fracture behaviour of fine-grained DP steels where shearing can contribute to severe elongation of dimples on the fracture surface, and shear fracture can lead to quasi-cleavage fracture, i.e. cleavage surfaces surrounded by dimples, as shown in Fig. 2.8.
2.2 Phenomenological damage models

The micro-scale deformation of dual phase steels is complex but at the macro-scale, it can be considered as a continuum. In continuum damage mechanics, the macroscopic response of materials is a global response of the material with its various constituents and defects. Phenomenological damage models usually assume an evolution of a phenomenological parameter based on homogenized variables like deformation gradient or velocity gradients to simulate materials behaviour. These models are computationally efficient and due to their relative simplicity, they are more widely-used in industrial applications [53].

2.2.1 Johnson-Cook model

Johnson and Cook [54] proposed a phenomenological damage model to predict the critical fracture strain as an extension to Hancock and Mackenzie’s [55] model as a function of equivalent plastic strain ($\varepsilon_p$), strain rate ($\dot{\varepsilon}_p$), temperature ($T$) and stress triaxiality ($\eta$). The JC progressive damage model considers that the damage accumulates incrementally in a linear way in the material element during a forming
process, as shown in Eq. 2.2a, and accelerates sharply when the damage increases over a critical value \[56, 57\]. \(D\) is defined as the damage variable and can change from 0 to 1 (Eq. 2.2b) which shows no damage and fully damaged material element, respectively \[56, 58\]. After the damage commences, the material stiffness and consequently, the load bearing capacity of the element decreases progressively until the final material failure. The relation between the accumulative damage parameter \((D)\), equivalent plastic strain \((\varepsilon_p)\) and critical plastic strain at the final fracture \((\varepsilon_f)\) is given by:

\[
D = \sum \frac{\Delta \varepsilon_p}{\varepsilon_f} \tag{2.2a}
\]

\[
\dot{D} = \begin{cases} 
0 & \text{if } \varepsilon_p < \varepsilon_d \\
\frac{D_c}{\varepsilon_f - \varepsilon_d} & \text{if } \varepsilon_p \geq \varepsilon_d \end{cases} \tag{2.2b}
\]

where \(\dot{D}\), \(D_c\) and \(\varepsilon_d\) are the damage rate, critical damage variable and damage threshold strain, respectively. The general expression for the equivalent plastic strain at the onset of damage in the JC model \[54, 57, 58\] is written as follows:

\[
\varepsilon_f = [D_1 + D_2 \exp(D_3 \eta)] \left[1 + D_4 \ln \left(\frac{\varepsilon_p}{\varepsilon_0}\right)\right] [1 + D_5 T^*] \tag{2.2c}
\]

where \(D_{1...5}\) are material dependent constants which need to be determined based on the dynamic behaviour of the material. \(\varepsilon_0\) and \(T^*\) are a reference strain rate and the homologous temperature, respectively. This fracture criterion is implemented in most of the well-known commercial finite element simulation software such as ABAQUS and LS-DYNA \[58, 59\]. This damage model was extensively utilized and reported in the literature to simulate the forming and damage behaviour of different engineering materials: Gillard et al. \[28\] and Hassannejadasl et al. \[29\] used it to evaluate the forming and damage behaviour of dual phase steels subjected to electro-hydraulic free forming (EHFF) and die forming (EHDF); the performance of this model as a phenomenological damage model and the Gurson-Tvergaard-Needleman (GTN) \[60, 61\] micromechanical damage model was assessed in multi-stage tube
hydropiercing; also Wierzbicki et al. [62] evaluated its capabilities and compared it to 5 other phenomenological damage models and concluded that it would be suitable for situations where the stress triaxiality changes in very narrow ranges.

2.2.2 MMC model

Usually, a phenomenological fracture model is a function of accumulative plastic strain and can describe the damage accumulation with stress triaxiality evolution. The original Mohr-Coulomb (MC) damage criterion which was commonly employed in soil and rock mechanics, has been modified by Bai and Wierzbicki to take both triaxiality and Lode angle into account in the prediction of the damage in ductile metals [63–66]. The three-parameter modified Mohr-Coulomb (MMC) fracture model is shown to be more effective than other widely-used phenomenological damage models in the literature [66] and used extensively in recent publications [67–69].

The first invariant of the Cauchy stress tensor ($I_1$) as well as the second and third invariants of the deviatoric stress tensor ($J_2, J_3$) are shown in the first three equations in Eq. 2.3. The von Mises equivalent stress can be defined as a function of $J_2$ (Eq. 2.3d) and the stress triaxiality ($\eta$), defined as the dimensionless hydrostatic pressure, can be calculated via Eq. 2.3e. In addition, the Load angle ($\theta$) and the dimensionless Lode angle parameter ($\bar{\theta}$) are directly related to normalized $J_3$ and are defined by Eq. 2.3f and Eq. 2.3g, respectively. Since $\eta$ and $\theta$ incorporate the effect of all mentioned invariants, any damage model, such as MMC which takes these two parameters into account, can be good representations of stress states [4].
\[ I_1 = tr(\sigma_{ij}) \quad (2.3a) \]
\[ J_2 = \frac{1}{2} S_{ij} S_{ij} \quad (2.3b) \]
\[ J_3 = det(S_{ij}) \quad (2.3c) \]
\[ \sigma_{eq} = \sqrt{3J_2} \quad (2.3d) \]
\[ \eta = \frac{\sigma_m}{\sigma_{eq}} \quad (2.3e) \]
\[ \theta = \frac{1}{3} \cos^{-1}\left(\frac{3\sqrt{3}}{2} \frac{J_3}{J_2^{3/2}}\right) \left(0 \leq \theta \leq \frac{\pi}{3}\right) \quad (2.3f) \]
\[ \bar{\theta} = 1 - \frac{6\theta}{\pi} (-1 \leq \bar{\theta} \leq 1) \quad (2.3g) \]

Bai and Wierzbicki [64, 65] developed the new form of the MMC fracture criterion by transforming the stress-based Mohr–Coulomb failure criterion into the space of stress triaxiality, Lode angle parameter and equivalent plastic strain. The final functional form of MMC fracture locus is given by:

\[
\bar{\varepsilon}_f(\eta, \bar{\theta}) = \left\{ \frac{A}{C_2} \left[ C_3 + \frac{\sqrt{3}}{2} - \sqrt{3}(1 - C_3) \left( \sec \left( \frac{\bar{\theta}\pi}{6} \right) - 1 \right) \right] \right. \\
\times \left. \left[ \sqrt{\frac{1 + C_1^2}{3}} \cos \left( \frac{\bar{\theta}\pi}{6} \right) + C_1 \left( \eta + \frac{1}{3} \sin \left( \frac{\bar{\theta}\pi}{6} \right) \right) \right] \right\}^{\frac{1}{n}} \quad (2.3h)
\]

where \( A \) and \( n \) are Swift law [70] hardening parameters, and \( C_{1...3} \) are material constants which should be determined by fracture tests. Luo and Wierzbicki [4] presented the 3D and 2D representation of the MMC fracture locus for DP780 (Fig. 2.9) which shows the ability of this model to predict the evolution of fracture stress with respect to both triaxiality and Lode angle.
In the case of plane strain deformation, the MMC fracture criterion can be reduced to a simpler form [71]:

\[
\bar{\varepsilon}_f = \left\{ \frac{AC_3}{C_2} \left[ \sqrt{\frac{1 + C_1^2}{3}} + C_1 \eta \right] \right\}^{(1/n)}
\]  

(2.3i)

2.2.3 GISSMO model

The generalized incremental stress-state dependent damage model (GISSMO) is a phenomenological damage model proposed by Neukamm et al. [72] which was established based on a combination of incremental material instability, failure criterion and localization. In this model, the failure description and the deformation path dependency of instabilities are included [73]. The final version of this model has been implemented in LS-DYNA finite element simulation software under the MAT_ADD_EROSION keyword [74]. The GISSMO model is described as a very pragmatic model which relies on both damage and regularization [74]. The regularization concept in this model refers to the mesh size dependency of the failure prediction via defining some material parameters as a function of element size. In order to take the arbitrary strain path into account
for prediction of localization and failure, the accumulative damage variable \((D)\) is considered as a generalized function of the linear accumulation of damage \([72, 75]\) proposed by Johnson and Cook \([54]\), as shown in Eq. 2.4a.

\[
\Delta D = -\frac{n\Delta \varepsilon_p D}{\varepsilon_f} \left(1 - \frac{1}{n}\right)
\]  

(2.4a)

\(\varepsilon_f\) is the triaxiality dependent failure strain. Similar to most phenomenological damage models, an element loses its load bearing capacity and should be omitted from the mesh when \(D\) reaches a critical value \((D_f=1)\). The main differences between GISSMO the Johnson-Cook damage model are: (1) the linear function used in JC model to describe damage accumulation is modified by a non-linear exponential function \((n=1\) in Eq. 2.4a results in linear JC formulation), and (2) the required data to calibrate this model is the equivalent plastic strain at failure as a function of triaxiality \([76]\). Since a non-linearity exists between the damage and equivalent plastic strain \([75, 77]\), even for proportional strain paths, it is hard for researchers to directly measure the model parameters through direct mechanical testing. Instead, reverse engineering simulations of multi-stage forming processes should be carried out to identify parameters of the non-linear relation of accumulation of damage. Similar to the damage parameter, the “forming intensity parameter \((F)\)” (as shown in Eq. 2.4b) follows the same non-linear incremental evolution where the accumulation exponent is greater than 1 \((n \geq 1)\). Figure 2.10 shows the evolution of \(F\) as a function of equivalent plastic strain from \(\varepsilon_f=0.68\).

\[
\Delta F = -\frac{n\Delta \varepsilon_p F}{\varepsilon_f} \left(1 - \frac{1}{n}\right)
\]  

(2.4b)
With regards to the material instability, a damage threshold should be defined, i.e. when the damage parameter $D$ reaches the critical threshold value, the damage gets coupled with the stress tensor and the effective stress tensor is calculated (Eq. 2.4c).

$$\sigma_{eq} = \sigma \left[ 1 - \left( \frac{D - D_c}{1 - D_c} \right)^m \right] \text{ for } D \geq D_c \quad (2.4c)$$

The effect of element size-dependency of the material behaviour can be introduced to the model via $m$ as the fading exponent. With this exponent, the effect of dissipated energy during element fade out, i.e. the process in which an element loses its load bearing capacity, can be controlled \cite{72, 78, 79}.

### 2.3 Micromechanical damage models

The damage accumulation process in heterogeneous materials is a complex process in multi-phase material structures due to grain size, second phase particles and precipitates and voids. The main mechanisms of ductile failure generally consist of nucleation, growth and coalescence of micro-voids during the forming process \cite{7, 43} in a porous media, although the fracture mechanism can vary from a shear mechanism at negative stress triaxialities to a combination of shear and void formation at low triaxialities \cite{80}. Therefore, micromechanical damage models which account for
these mechanisms are more suitable to numerically evaluate ductile failure in metal forming simulations, although it is shown that it is hard to define a damage model that can predict the ductile fracture for different triaxiality levels \[81\]. Since various combinations of void size, shape, spacing and orientation can be made to analyse the ductile fracture in a material, simplifications and assumptions have to be considered to make the mathematical evaluation of void evolution feasible. Accordingly, some models considered cylindrical or spherical shapes for the voids \[61, 82–84\]. Also, complete loss of load bearing capacity of the material cell or the final failure occurs when the size or the total volume fraction of voids reaches a critical value \[85\].

### 2.3.1 McClintock model

McClintock \[82\] proposed a model for void growth and ductile fracture based on a long cylindrical void in a non-hardening material pulled in the axis direction while subjected to transverse tensile stresses. The growth of the cylindrical cavity is given by

\[
d\log \frac{b}{b_0} = \sqrt{3} \sinh \left( \frac{\sqrt{3} \sigma_r}{\sigma_r - \sigma_z} \right) d\varepsilon_r + d\varepsilon_r \tag{2.5a}
\]

where \(z\) and \(r\) denote the axial and radial directions, respectively. \(b_0\) is the original radius of the cylindrical cavity and \(b\) is its instant value. He assumed a 3D array of cylindrical voids of elliptical section in which the main axes are parallel to the principal stress axes. Considering the main axis of the cylindrical void parallel to the \(z\) direction, McClintock extrapolated Berg’s viscous solution \[86\] for elliptical voids to plastic materials with strain hardening if the voids grow in the \(b\) direction and expressed his fracture criterion in the following form:

\[
\frac{d\eta_{zb}}{d\varepsilon_p} = \frac{\sinh \left[ \frac{(1-n)(\sigma_a + \sigma_b)}{2\sigma_{eq}/\sqrt{3}} \right]}{(1-n)\ln F^{t}_{zb}} \tag{2.5b}
\]
where $d\eta_{zb}$ is the damage increment and $\frac{d\eta_{zb}}{d\varepsilon_p}$ denotes the damage rate. $F_{zb}^f$ represents the critical value of the relative growth factor or the maximum sustainable deformation of the representative cell. $\sigma_{a,b}$ are two principal stresses in transverse directions. The main outcomes of the McClintock model are the strong dependency of the fracture strain to the tensile strength transverse to the void main axis, and relative sensitivity of the fracture strain on the intermediate principal stress rather than solely to the maximum principal stress [82, 85]. Although this model shows some fundamental features of ductile fracture the effect of triaxiality to reduce the fracture strain and the size effect, the simplifications in this model lead to unrealistic results. It predicts void growth as a smooth process up to final failure whereas the loss of stability results in sudden void growth and coalescence [87–89].

2.3.2 Rice-Tracey model

One of the most famous void growth related functions was proposed by Rice and Tracey [83]. This model evaluates the dilatational growth of a single spherical void in a non-hardening material subjected to a remote uniaxial stress field. They showed that the void would grow in the radial direction and its shape would also alter. The classical equation for growth rate of void radius under a high triaxiality stress state is given by:

$$\frac{dR}{R} = \alpha_{RT} \exp\left(\frac{3}{2} \eta\right) d\varepsilon_p$$

(2.6a)

where $\eta$ is the stress triaxiality (shown in Eq. 2.3e) and $R$ is the current radius of the spherical void. $\alpha_{RT}$ is the Rice and Tracy model constant and equals 0.283. The RT model predicts the growth of a void or a population of identical cavities as a linear function of the equivalent plastic strain increment. It is shown that the void growth rate is underestimated in this model when utilizing $\alpha_{RT}$. Also, hard inclusions and second phases inside a growing cavity are likely to accelerate the growth rate [90, 91]. Later, Huang found that $\alpha_{RT}$ is more applicable to stress states in which $\eta > 1$. Therefore, he modified the original RT model by adjusting the constant ($\alpha_{Huang} = 0.427$)
and adding a stress triaxiality term to calculate the average rate of void growth for $\eta \leq 1$:

$$\frac{dR}{R} = \left\{ \begin{array}{ll}
\alpha_{Huang} \eta^{1/4} \exp \left( \frac{3}{2} \eta \right) d\varepsilon_p & \text{if } \eta \leq 1 \\
\alpha_{Huang} \exp \left( \frac{3}{2} \eta \right) d\varepsilon_p & \text{if } \eta > 1
\end{array} \right. \quad (2.6b)$$

Equation (2.6b) has been widely used in several publications to investigate void growth using X-Ray tomography analysis in different materials [46 92 93] especially dual phase steels [46 47 94 95]. Void nucleation has been modelled with different types of functions based on stress or strain states. However, since the stages of ductile damage can happen simultaneously and affect each other, the RT model needs to be modified to take the influence of void nucleation on the void growth into account. This modification was performed by different researchers [45 93 95] and is given by:

$$\frac{dR}{d\varepsilon_p} = \alpha_{RTm} \exp \left( \frac{3}{2} \eta \right) R - \frac{1}{N} \times \frac{dN}{d\varepsilon_p} (R - R_0) \quad (2.6c)$$

where $R_0$ is the radius of voids just after their nucleation, and $dN$ and $N$ are the nucleation rate and the void density respectively. It should be noted that the RT model is not capable of predicting damage evolution or the fracture strain in pure shear, where $\eta = 0$.

### 2.3.3 Gurson-Tvergaard-Needleman model

Gurson [60 84] proposed a new methodology and introduced a yield function for a material containing voids that could link the plasticity with the damage accumulation by applying maximum plastic work principle to kinematically admissible velocity fields for a long cylindrical or spherical void in a continuum [96 97]. He stated that in the presence of voids in a material, the load carrying capacity would reduce and the material would soften as the porosity volume ($f$) increases. The yield function for
spherical voids in an isotropic rigid-plastic body is written as:

$$\Phi_p = \frac{\sigma_{eq}^2}{\sigma_y^2} + 2f \cosh \left( -\frac{3 \sigma_m}{2 \sigma_y} \right) - 1 - f^2 = 0 \quad (2.7a)$$

$$\dot{f} = \dot{f}_g + \dot{f}_n \quad (2.7b)$$

where $\sigma_{eq}$ and $\sigma_y$ denote the macroscopic von Mises equivalent Cauchy stress and yield stress of the fully dense matrix, initially equal to $\sigma_0$ (initial yield stress). $f$ defines the void volume fraction. The change in void volume fraction ($\dot{f}$) is described by the growth rate of existing voids ($\dot{f}_g$) and the secondary void nucleation rate ($\dot{f}_n$). When $f=0$, Eq. (2.7a) is equal to the von Mises yield criterion. The original form of the Gurson model represents only the damage growth and it is shown that without an initial imperfection, it overpredicts the strain at which localisation commences. To reduce this discrepancy and minimize the difference between the model and finite element cell results, Tvergaard et al. [61, 98, 99] introduced new damage parameters ($q_1$, $q_2$ and $q_3$) into the Gurson yield function which has led to the so-called GTN model (Gurson–Tvergaard–Needleman) model:

$$\Phi_p = \frac{\sigma_{eq}^2}{\sigma_y^2} + 2q_1f \cosh \left( -\frac{3 q_2 \sigma_m}{2 \sigma_y} \right) - 1 - q_3 f^2 = 0 \quad (2.7c)$$

where $q_1$, $q_2$ and $q_3$ are material constants equal to 1.5, 1 and $q_1^2$ although it was demonstrated that these parameters are dependent on the triaxiality level [100, 101]. The GTN model is perhaps the most well-known micromechanical damage model and different researchers have either extended or modified it in order to make it as accurate as possible. Gologanu et al. [102] have included void shape in the GTN model and Benzerga et al. [103] extended this model by introducing two material parameters in the yield function to take the plastic anisotropy into account. Leblond et al. [104] used two new parameters to include isotropic hardening and plastic hardenable hollow sphere in the model. Finally, Mear and Hutchison [105] extended the GTN constitutive damage model to account for the kinematic hardening. The GTN model has been
extensively used to simulate the deformation and damage behaviour of DP steel under different strain paths and deformation modes using isotropic or kinematic hardening and plastic anisotropy.

2.3.4 Rousselier model

Rousselier proposed a thermodynamically consistent ductile damage models using the ‘simplest assumption’ at each stage of its development. It is an an elasto-plastic, continuous damage model that assumes isotropic-hardening and isotropic-damage to model ductile failure mechanism of porous materials during the deformation of a material. It is established based upon the decomposition of the free Helmholtz potential energy ($\Phi$) into stored elastic energy ($\Phi_e$), stored plastic energy ($\Phi_p$) and stored damage energy ($\Phi_d$), and is written as

$$\Phi(\varepsilon_e, \varepsilon_p, f) = \Phi_e(\varepsilon_e) + \Phi_p(\varepsilon_p) + \Phi_d(f)$$  \hspace{1cm} (2.8a)$$

where $\varepsilon_e$, $\varepsilon_p$ and $f$ are the elastic strain, plastic strain and the volume fraction of the current porosities, respectively. The plastic potential, proposed by Rousselier, is an extension of the von Mises yield criterion with an additional term which describes the damage as the growth of voids in a ductile material:

$$\Phi = \frac{\sigma_{eq}}{(1 - f)} - H(\varepsilon_p, \dot{\varepsilon}_p) + B(\beta)D \exp\left(\frac{\sigma_m}{(1 - f)\sigma_k}\right) = 0$$  \hspace{1cm} (2.8b)$$

in which $\sigma_{eq}$ is the von Mises equivalent stress (such that $\sigma_{eq} = (\frac{1}{2}S_{ij}S_{ij})^{1/2}$ where $S_{ij}$ is the deviatoric stress) and $\sigma_m$ is the hydrostatic stress (such that $\sigma_m = \frac{1}{3}tr(\sigma_{ij})$ where $\sigma_{ij}$ is the Cauchy stress). $D$ and $\sigma_k$ are material parameters which describe the resistance of the material to void growth and coalescence. $H(\varepsilon_p, \dot{\varepsilon}_p)$ is the hardening curve of the material which can be described either by hardening functions or tabular data; $B(\beta)$, the damage function, is the conjugate force to the damage parameter $\beta$. $f_0$ and $f$ are the initial and current void volume fraction, respectively. The damage variable $\beta$ and $f$ are directly related to the plastic multiplier in the
normality rule ($\lambda$) and follow the strain increment ($\dot{\varepsilon}_p$), increase with the deformation and help material softening surpass the hardening in the final steps of deformation until the material completely loses its load-bearing capacity:

\[
\dot{f} = (1 - f) \dot{\varepsilon}_p f D \exp\left(\frac{\sigma_m}{(1 - f)\sigma_k}\right) \quad (2.8c)
\]

\[
\dot{\beta} = \dot{\varepsilon}_p D \exp\left(\frac{\sigma_m}{(1 - f)\sigma_k}\right) \quad (2.8d)
\]

The relation between the damage parameter $\beta$, $f$ and the initial void volume fraction ($f_0$) is given by:

\[
\beta = \ln\left(\frac{f}{1 - f} \times \frac{1 - f_0}{f_0}\right) \quad (2.8e)
\]

and the current void volume fraction as a function of the damage function ($B$) is written as:

\[
f = \frac{B(\beta)}{\sigma_I} = \frac{f_0 \exp(\beta)}{1 - f_0 + f_0 \exp(\beta)} \quad (2.8f)
\]

Li et al. [112] presented an explicit and detailed theoretical calculation procedure of the Rousselier damage model and its related parameters. In the original Rousselier model, cluster nucleation model was used and the effect of secondary void nucleation was not considered. Therefore, void nucleation was defined by the fraction of second phase particles present in the material and void growth ($df_g$) was considered as the main mechanism for void evolution ($\dot{f}$), as shown in Eq. (2.8g). In addition, failure was described by specifying a critical void volume fraction ($f_c$) which corresponds with a critical value of the damage parameter $\beta_c$ [119, 120, 120].

\[
df = df_g, \quad f(0) = f_0 \quad (2.8g)
\]
The Rousselier damage model has been used in several publications to evaluate the deformation and damage behaviour of materials since it has two major advantages over the GTN damage model: (1) it requires fewer model constants to be defined, (2) it has the capability of predicting damage evolution and void volume fraction growth at very low, zero or negative stress triaxiality and (3) unlike the GTN model which defines the damage evolution in a material based on the growth of a spherical or cylindrical shaped void, the Rousselier damage model was developed without consideration of the shape of voids and accordingly, it can determine the damage transition from flat to slant fracture surface without any additional terms [113, 121]. Besson et al. [122] used the Rousselier function to model crack growth and formation of cup-cone fracture surfaces; Poussard et al. [123] employed it to simulate the damage evolution in smooth tensile and compact tension specimens. Samal and Shad [124] predicted the fracture resistance behaviour of cracked fuel pin specimens using this model; Tu et al. employed it to evaluate the ductile damage and crack growth on S355NL steel electron beam welded joints [125] and aluminium laser-welded joints [126]; and Zanganeh et al. [118] proposed an approach to couple the Rousselier model and a coalescence criterion and evaluated the model for different positive triaxiality levels using notched AA2050 specimens loaded in uniaxial tension.

2.3.5 Lemaitre model

Lemaitre [127–129] proposed an isotropic damage model based on the concept of damage variable \( (D) \) and its effect on the effective stress \( (\sigma_{eff} = \sigma_n / (1 - D)) \). Damage is considered as a thermodynamic state variable which is responsible for characterizing the deterioration of the material [66]. The change in the shape, number and volume fraction of voids in a porous ductile material lead to an increase in the damage parameter which results in decreasing the load-bearing capacity of the material cell. On an intersection of a reference volume element with a plane \( (S) \) with the normal vector \( \vec{n} \), the damage variable is defined as:

\[
D_n = \frac{S^n_0 - S^n_{ef}}{S^n_0} \tag{2.9a}
\]
where $D_n$ is the damage variable in the direction of the normal vector $n$, and $S_{ef}^n$ and $S_0^n$ represent the effective resisting area of the intersection plane and the nominal intersection area of the plane and the reference volume prior to the onset of damage, respectively. Since the Lemaitre damage model considers an isotropic distribution of damage, the value of the damage variable is the same in all directions and $D$ (a scalar factor) can be utilized instead of $D_n$. Generally, the damage variable is linearly related to the equivalent plastic strain, deduced from the damage dissipation potential and the damage strain strain energy release rate \[127\]. The general constitutive equation for ductile plastic damage is given by:

$$
\dot{D} = \left\{ \frac{K^2}{2ES_0} \left[ \frac{2}{3} (1 + \nu) + 3(1 - 2\nu) \left( \frac{\sigma_m}{\sigma_{eq}} \right)^2 \right] \dot{\varepsilon}^{2/n} \right\} \dot{\varepsilon}_p \tag{2.9b}
$$

where $K$ and $n$ are constants in the Ramberg-Osgood hardening law (as shown in Eq. 2.9c).

$$
\varepsilon_p = \left( \frac{\sigma_{eq}}{k} \right)^n \tag{2.9c}
$$

An advantage of the Lemaitre continuous damage model is that it can be utilized for any damage process, not just ductile damage \[119\] \[130\]. In addition, the damage evolution equation can be solved by any relevant constitutive elasto-plastic equation for a damaged material \[66\] \[131\] as it has also been modified by Niazi \[19\] to include anisotropy.

### 2.4 Brittle damage models

Brittle fracture is a damage mode that has extensively been studied by different researchers. The effective factors, different theories and mathematical models were developed to numerically and experimentally investigate this phenomenon at both micro- and macro-levels \[132\] \[133\]. Moreover, several fracture criteria were proposed
to evaluate the onset of fracture, fracture toughness and fracture angle \[132, 134, 140\].
A number of reviews of brittle fracture can be found in the literature \[119, 132\].

### 2.4.1 Crack nucleation

It is generally accepted that cleavage fracture in mild steel starts from a localization of stress in the material due to a dislocation pile up at an obstacle \[136, 137\]. For slip-induced fracture, this critical stress is shown to be temperature and strain rate independent, but if the fracture is initiated by twinning processes, it is very sensitive to testing parameters \[136\]. The initiation of microcracks can also be a result of dislocation pile-ups at grain boundaries or at the interfaces between dissimilar phases which results in cleaving a grain boundary \[132, 141\]. A widely-used cleavage fracture criterion is written as follows \[142, 143\]:

\[
\begin{align*}
\sigma_{eq} & \geq \sigma_y \quad (2.10a) \\
\sigma_I & \geq \sigma_f \quad (2.10b)
\end{align*}
\]

where \(\sigma_{eq}\), \(\sigma_y\) and \(\sigma_I\) are the von Mises equivalent stress, material yield stress and maximum principal stress, respectively. \(\sigma_f\) represents the critical brittle fracture stress or cleavage fracture stress.

It has been shown that the nucleation of cracks occurs in carbide particles or other brittle phases after some amount of plastic deformation in the ferrite. However, dynamic crack propagation within a brittle second phase or a carbide creates a stress field within the second phase that is predominantly in shear and would not result in significant plastic deformation in ferrite. The cleavage crack can thus propagate dynamically across the interface if \(\sigma_I\) exceeds the effective particle strength for a particle size of \(d_p\)\[138, 141, 144, 145\].

\[
\sigma_f = \left[ \frac{\pi E G_{cf}}{2 (1 - \nu^2) d_p} \right]^{1/2} \quad (2.10c)
\]
where $E$, $\nu$ and $G_{cf}$ are Young’s modulus, Poisson’s ratio and critical strain energy release rate for the dynamic propagation of a crack into the ferrite matrix. If $\sigma_f > \sigma_I$ or if the crack reaches a high angle misorientation grain boundary, the crack would be arrested at the grain boundary $\textbf{141, 146, 147}$. Continued extension of the crack across ferrite-ferrite boundaries takes place when the maximum principal stress exceeds the ferrite grain strength which can be similarly described as a function of the ferrite grain size ($d_g$) and effective surface energy of the ferrite-ferrite interface ($G_{ff}$):

$$\sigma_{ff}^f = \left[ \frac{\pi E G_{ff}}{2 (1 - \nu^2) d_g} \right]^{1/2}$$

(2.10d)

The concept of “critical distance” was introduced by Ritchie et al. $\textbf{148}$ who suggested that the maximum principal stress should be greater than the critical cleavage stress ($\sigma_f$) over a distance of one or two grain sizes ahead of the crack tip in order to cause the crack to propagate $\textbf{132}$.

**Weakest link**

The weakest link statistical model was used by several researchers to analyse the propagation of microcracks in a particle into the matrix grains as a critical step for cleavage fracture $\textbf{141, 145, 149, 150}$. In this model a certain volume ($V$) which represents the plastic zone, is discretized into elements with constant tensile stress which should resist and avoid the cleavage fracture. Therefore, the total survival probability of the entire microstructure can be calculated by integration of the survival probabilities of all elements over $V$ $\textbf{141, 151}$:

$$\Phi = 1 - \exp \left[ \int_0^V \int_0^\sigma g(S) dS \right]$$

(2.11a)

where $g(S) dS$ is the number of cracked particles or microcracks per unit volume ($V_0$) with strengths between $S$ and $S + dS$. Usually, a three-parameter Weibull probability
distribution expression is a convenient way to define $g(S) \, dS$:

$$
\int_{0}^{\sigma} g(S) \, dS = \left( \frac{\sigma - \sigma_{th}}{\sigma_u} \right)^m
$$

(2.11b)

where $m$ is the shape parameter, $\sigma_u$ is the scale parameter or lower bound strength, and $\sigma_{th}$ is the offset parameter which is a threshold stress needed for the largest feasible microcrack to propagate. Beremin [152] used the concept of the weakest link to analyse eligible particles that participate in the fracture process. Satisfaction of both crack nucleation and crack propagation are the main requirements to determine the eligibility of particles. The criterion proposed by Beremin is expressed as a probability distribution based on Weibull theory [152, 153]:

$$
\begin{align*}
P_R &= 1 - \exp \left[ - \left( \frac{\sigma_w}{\sigma_u} \right)^m \right] \\
\sigma_w &= \left[ \frac{1}{V_0} \int_{0}^{V} (\sigma_I - \sigma_{th}) \, dV \right]^{1/m}
\end{align*}
$$

(2.11c)

where $P_R$ is the cumulative probability of failure and $\sigma_w$ denotes the Weibull stress which is considered to be independent of temperature.

### 2.4.2 Folch

Folch and Burdekin [154] proposed coupled brittle-ductile model based on a combination of modified Beremin and Lemaitre models. According to this approach, the integration process in Eq. 2.11c is carried out over a volume of material within a cell, i.e. $V_0 = V$. Therefore the threshold stress ($\sigma_{th}$) becomes zero and the Weibull stress ($\sigma_w$) equals the maximum principal stress. Accordingly, Eq. 2.11c can be re-written as [154, 155]:

$$
\Phi = 1 - \exp \left[ - \left( \frac{\sigma_I}{\sigma_u} \right)^m \right]
$$

(2.12)
Since the probability of cleavage fracture and the material constitutive response are determined simultaneously in Folch’s model, both brittle and ductile fracture mechanisms can be modelled and evaluated at the same time. Good agreement between the results of Charpy tests and the predicted fracture toughness was reported [154, 155].

2.5 Hardening constitutive functions

In the modelling of metal forming processes or crash simulations, hardening and softening of the sheet material are dependent on thermomechanical parameters derived from experimental flow curves. Therefore, it is important to carefully determine the parameters in a hardening equation, whether it is a phenomenological, physically-based or artificial neural network model [156], so that the mechanical behaviour of the sheet material can be accurately predicted. Since ductile metals and alloys can be safely deformed up to high strain values, the formulation of these equations in terms of predicting hardening behaviour and hardening rate is critical [157, 158].

In the following sections, $C_1...n$ are materials constants which can be determined by an appropriate fitting procedure and $H, \varepsilon_p, \dot{\varepsilon}_p$ and $T$ denote the material flow stress, the equivalent plastic strain, the equivalent plastic strain rate and temperature, respectively. A number of useful publications are available to review different hardening functions, their origins and their performance in different process conditions [156, 157].

2.5.1 Strain dependent models

A large number of hardening flow curve models are developed based on strain hardening parameters which fit quite well with the experimental true stress-true strain up to uniform elongation achieved by tension test. In the absence of an appropriate mechanical test such as hydrostatic bulge test, extrapolation of the predicted hardening curve at high strain levels differs, depending on the nature of the model. In some functions such as 3-parameter Voce model (Eq. 2.13c) [159], the flow stress is limited to a saturated value ($\sigma_s$) and the strain hardening rate ($d\sigma/d\varepsilon_p$) becomes naught after
uniform elongation. Other models such as the power law (Eq. 2.13a), Ludwik’s law (Eq. 2.13a) and the 4-parameter Voce law take stage IV hardening of the material into account, and predict a non-zero hardening rate at high strains. The first group are called saturated-type hardening functions and the second group are described as unbounded-hardening models. Among the latter group, different models predict the slope of the hardening curve as linear (4-parameter Voce) or non-linear (power law, Ludwik’s). Although these models are widely used in the literature, other hardening functions such as Swift-Voce, El-Magd, generalized Voce and Bergström were developed to optimize the behaviour of the model and increase its accuracy.

\[
H(\varepsilon_p) = C_1 \left( \frac{\varepsilon_p}{E} + 1 \right) \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_3} 
\]

\[
H(\varepsilon_p) = C_1 + C_2 \varepsilon_p^{C_3} 
\]

\[
H(\varepsilon_p) = C_1 - (C_1 - C_2) \left( 1 - \exp(-C_3 \varepsilon_p) \right) 
\]

\[
H(\varepsilon_p) = C_1 - (C_1 - C_2) \left( 1 - \exp(-C_3 \varepsilon_p) \right) + C_4 \varepsilon_p 
\]

2.5.2 Rate and temperature dependent models

The dynamic behaviour of materials in a wide range of strain rates, from quasi-static conditions to high strain rates (≥1000 s\(^{-1}\)), and forming temperature becomes of interest of both academia and industry since sheet materials can be deformed under such a wide range of conditions. Different hardening models can be found in the literature based on strain-rate or temperature dependency of the material hardening behaviour. Advanced high strength steels show some strain-rate sensitivity. Therefore, an accurate hardening function should be chosen to describe the overall strain rate, temperature and strain dependency of flow curves analytically. Usually, the experimental flow curves are fitted by an optimisation algorithm in order to achieve the best fitting result. Model parameters instead of experimental flow curves are then given as input data for FE simulations.
As mentioned in Section 2.5.1 different types of hardening models are proposed in the literature to model the static or dynamic hardening behaviour of materials. Power law-type models such as Johnson-Cook (JC) (Eq. 2.14a) and modified Johnson-cook hardening (Eq. 2.14b) models 170,171, Zirilli–Armstrong (ZA-BCC) (Eq. 2.14e) 172, Khan–Huang–Liang (KHL) model (Eq. 2.14d) 173,175 are suitable for body-centered cubic (BCC) materials at low temperatures 176 while Voce-type models such as Brown–Anand (BA) 177,178, MTS model 179, Lin-Wagoner (LW) model 180, and ZA-FCC (Eq. 2.14f) are found to be more appropriate for face-centred cubic (FCC) metals and alloys 181. Some constitutive hardening models were developed based on multiplicative or additive (or both) combinations of strain, strain rate and temperature dependent functions 171 such as JC and El-Magd-Swift (Eq. 2.14c) 166 models, and other so called “integrated” models were developed based on their approach in accommodating strain hardening rate changes with temperature changes. A number of review books and papers have been published on the constitutive descriptions for metals and alloys in cold and hot working 156,157,182.

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = (C_1 + C_2 \varepsilon_p^{C_3}) \left[ 1 + C_4 \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right) \right] \left[ 1 - \left( \frac{T - T_0}{T_m - T_0} \right)^{C_5} \right] \quad (2.14a)
\]

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = (C_1 + C_2 \varepsilon_p^{C_3}) \left[ 1 + C_4 \left( \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \right] \left[ 1 - \left( \frac{T - T_0}{T_m - T_0} \right)^{C_6} \right] \quad (2.14b)
\]

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = \left[ C_1 (C_2 + \varepsilon_p)^{C_3} + C_4 \dot{\varepsilon}_p \right] \exp \left( -C_5 \frac{T - T_0}{T_m} \right) \quad (2.14c)
\]

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = \left[ C_1 + C_2 \left( 1 - \frac{\ln \dot{\varepsilon}_p}{\ln D_p} \right)^{C_4} \varepsilon_p^{C_5} \right] \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \left( \frac{T_m - T}{T_m - T_{ref}} \right)^{C_6} \quad (2.14d)
\]

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = C_0 + C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}_p) + C_5 \varepsilon_p^{C_6} \quad (2.14e)
\]

\[
H(\varepsilon_p, \dot{\varepsilon}_p, T) = C_0 + C_1 \varepsilon_p^{0.5} \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}_p) \quad (2.14f)
\]
2.6 Void nucleation functions

The onset of ductile fracture is initiated by the growth of existing voids and the formation of new secondary voids around inclusions or second-phase particles in the metal matrix during the forming process due to the external loading. Therefore, the increase in the void volume fraction is a result of both void growth and void nucleation. For some engineering materials with easy-to-break inclusions, such as aluminium oxides, voids are nucleated at the beginning stages of deformation. In this condition, the cluster nucleation function assumes an initial void volume fraction \( f_0 \) and no secondary void nucleation is considered (Eq. 2.15a). The cluster nucleation model has been used to simulate the damage behaviour of aluminium and steel. Continuous nucleation model is a simple model which does take the secondary void nucleation into account which is appropriate for materials containing carbides or intermetallic phases. In this model, void nucleation is linearly proportional to the increment of plastic strain, as shown in Eq. 2.15b and it has been shown that it can be a realistic model for both steel and aluminium alloys.

\[
df_{\text{nucleation}} = 0 \quad \text{and} \quad f_{t=0} = f_0 \\
df_{\text{nucleation}} = C \, d\varepsilon_p
\]

Beyond these simple models, it has been shown that employing a void nucleation function that is controlled either by strain, stress or hydrostatic stress, can make a model more precise and more realistic \( df = df_g + df_N \). Generally, hydrostatic stress controlled nucleation (Eq. 2.16d) is used for rubber-modified epoxies, stress-controlled void nucleation is used for materials with large particles that tend to crack (Eq. 2.16c), and strain-controlled void nucleation (Eq. 2.16b) is more suited to materials with small particles that tend to debond from the matrix. Although both strain and stress-controlled nucleation models can be used for DP600 due to the size of its martensite particles, both Butcher et al. and Ramazani et al.
[6] showed that strain-controlled void nucleation could lead to more accurate results compared to cluster nucleation. The general form of the controlled void nucleation function can be written as:

\[
df_{\text{nucleation}} = A \, d\sigma_{eq} + B \, d\sigma_m + C \, d\varepsilon_p
\]  

(2.16a)

\[
A = B = 0, \quad C = f_N \frac{\sigma_y}{\sqrt{2\pi} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{S_N} \right)^2 \right]}
\]  

(2.16b)

\[
A = \frac{f_N}{S_N \sigma_y \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\sigma_0 + \sigma_m - \sigma_N}{S_N \sigma_y} \right)^2 \right], \quad B = C = 0
\]  

(2.16c)

\[
A = 0, \quad B = \frac{f_N}{S_N \sigma_y \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\sigma_m - \sigma_N}{S_N \sigma_y} \right)^2 \right], \quad C = 0
\]  

(2.16d)

where \( A, B \) and \( C \) are material parameters; \( df_n \) is the first derivative of the porosity distribution with respect to time; \( f_N \) is the volume fraction of void nucleating particles. \( \sigma_N \) or \( \varepsilon_N \) denotes the mean value of the normal distribution function and \( S_N \) represents the standard deviation. Although Eqs. 2.16 are the most widely-used secondary void nucleation functions in the literature, other models have been proposed based on the microstructure of dual phase steels in which the void density \( N \) is a function of both triaxiality \( \eta \) and the macroscopic equivalent plastic strain [193, 194] and is given by:

\[
N = A \left( \frac{\varepsilon_p}{\varepsilon_N} \right) \exp \left( \frac{\varepsilon_p}{\varepsilon_N} \right)
\]  

(2.17a)

\[
\varepsilon_N = \varepsilon_{N0} \exp(-\eta)
\]  

(2.17b)

where \( A \) and \( \varepsilon_{N0} \) are a material constant and a critical strain for pure shear loading, respectively. In addition, Landron et al. [195] and Fansi et al. [26] employed a new
void nucleation law that defines the rate of the void density function \( N \) using:

\[
\frac{dN}{d\varepsilon_p} = B \sigma \left( \frac{\sigma}{\sigma_c} \right) \left( 1 + \eta \frac{\sigma}{\sigma - X} \right) \frac{f_N}{f_{N_0}} \tag{2.18}
\]

where \( B \) and \( N_0 \) are material constants and \( \sigma_c \) the critical shear stress value that the martensite-ferrite interface can support without breaking. In addition, \( \sigma \) and \( X \) denote the macroscopic values for stress and backstress, respectively.

### 2.7 Void coalescence criteria

Coalescence can be defined as the rapid linking of voids to build a microcrack in the material which contributes to a sudden decrease in the load-bearing capacity and final failure. It is the last of the three stages of the ductile fracture process (nucleation, growth and coalescence of voids). Different qualitative and quantitative models have been proposed based on mathematical concepts or experiments to make a better understanding of this phenomenon [77, 92, 95, 196–198].

McClintock [82] proposed a model for void growth and coalescence of cylindrical cavities based on an inverse relation of fracture strain and hydrostatic stress. His model takes the strain hardening behaviour into account in void growth and their impingement. Since it was developed for cylindrical or spherical voids and the interaction of voids has not been included in this model, it overestimates the fracture strain.

\[
\frac{dR}{R} = \frac{\sqrt{3} d\varepsilon_{eq}^p}{2(1 - n)} \sinh \left( \frac{(1 - n) \sigma_m \sqrt{3}}{\sigma_{eq}} \right) \tag{2.19}
\]

A geometrical model based on void length and spacing was proposed by Brown and Embury [199, 200] in which the coalescence occurs when the void length becomes equal to the intervoid spacing. So, the mean planar spacing \( \lambda \) of spherical particles with mean diameter \( d \) and volume fraction \( V_f \) is defined by Eq. 2.20a. Accordingly,
the fracture strain \((\epsilon_f)\) is given by Eq. 2.20b

\[
\lambda = \frac{1}{2} d \left( \sqrt{\frac{2\pi}{3 V_f}} - \sqrt{\frac{8}{3}} \right) \tag{2.20a}
\]

\[
\epsilon_f = \ln(1 + \epsilon_g + \epsilon_n) = \ln \left( \sqrt{\frac{\pi}{6 V_f}} - \sqrt{\frac{2}{3} + \epsilon_n} \right) \tag{2.20b}
\]

where \(\epsilon_n\) and \(\epsilon_g\) are the strain at which a void nucleates and grows to its critical size, respectively. Since this model does not include either hydrostatic stress, triaxiality component or material properties, it also overestimates the fracture strain. Le Roy \[201\] modified this model by adding stress triaxiality.

Needleman and Tvergaard \[61, 98, 99\] extended the original Gurson ductile damage model to include void coalescence and void growth acceleration towards final failure. In this model, a critical void volume fraction \((f_c)\), considered to be a material constant, determines the onset of coalescence and sudden material capacity loss. However, it has been pointed out that \(f_c\) strongly depends on the initial void volume fraction \((f_0)\) and on the strain path \[188\].

\[
f_c = \text{const.} \tag{2.21}
\]

The plastic limit-load model (PLL) was proposed by Thomason \[89, 191\] to predict the localized plastic failure of the intervoid matrix and has become an acceptable criterion for identifying the onset of coalescence. The concept of this model lies in two competitive modes of deformation: stable homogeneous and unstable localized. In the early stages of deformation, void volume fraction is low and it is easier to achieve homogeneous deformation. Nevertheless, the stress required for localized deformation decreases by void nucleation and growth during the deformation. Based on this criterion, when the stress required for homogeneous deformation and that of localized deformation become equal, coalescence occurs, the plastic limit-load is reached, the deformation will localize between neighbouring voids, and the current
void volume fraction can be considered as the critical void volume fraction at the onset of coalescence \( (f_c) \). Many researchers extended Thomason’s model to include the effect of material properties, cell geometry \[100, 202\] and void shape \[203\]. Zhang et al. \[188\] wrote the Thomason plastic limit-load criterion for a 3D deformation system as follows:

\[
\frac{\sigma_I}{\sigma_{eq}} \left[ \alpha_t \left( \frac{1}{\chi} - 1 \right)^2 + \frac{\beta_t}{\sqrt{\chi}} \right] (1 - \pi \chi^2) = \left( \frac{3f}{4\pi} \exp(\varepsilon_I + \varepsilon_{II} + \varepsilon_{III}) \right)^{1/3} \left( \frac{(\exp(\varepsilon_{II} + \varepsilon_{III}))^{1/2}}{2} \right)^{-1} \tag{2.22a}
\]

\[
\chi = \left( \frac{3f}{4\pi} \exp(\varepsilon_I + \varepsilon_{II} + \varepsilon_{III}) \right)^{1/3} \left( \frac{(\exp(\varepsilon_{II} + \varepsilon_{III}))^{1/2}}{2} \right)^{-1} \tag{2.22b}
\]

where \( \sigma_I \) is the maximum principal stress, \( \alpha \) and \( \beta \) are model constants, \( \chi \) represents the void space ratio, and \( \varepsilon_{I,II,III} \) denote principal strains. Another representation of Thomason’s model can be found in Pardoen et al. \[202\] and Scheyvaerts et al. \[204\]:

\[
\frac{\sigma_I}{\sigma_{eq}} = \left[ \alpha_t \left( \frac{1}{W \chi} - 1 \right)^2 + \frac{\beta_t}{\sqrt{\chi}} \right] (1 - \eta \chi^2) \tag{2.23}
\]

where \( W \) and \( \eta \) are the void aspect ratio \( (W=1 \) for spherical voids) and a geometric factor based on void arrangement and void cell geometry \( (\eta=1 \) for cylindrical cell geometry), respectively. Although \( \alpha_t \) and \( \beta_t \) were defined as constants in Thomason’s original model, Pardoen and Hutchinson \[100\] redefined the former parameter as a function of the strain hardening exponent \( n \) in the power law hardening function in order to take the hardening behaviour of the material into account. Their calculations based on large numbers of axisymmetric finite element cell calculations indicated that \( \alpha_t = 0.1 + 0.217n + 4.83n^2 \) for materials with \( 0 \leq n \leq 0.3 \) and \( \beta_t \approx 1.24 \).

Another approach to calculate the void space ratio, i.e. the ligament size ratio \( (\chi) \) was proposed by Chambert et al. \[205\] based on a cylindrical unit cell with a height \( 2H \) units and a base of radius \( R \) units, which contains a spherical void with radius \( r \). Initial values for the height and radius of the cell are \( H_0 \) and \( R_0 \), respectively.
Combined with a unit cell aspect ratio \( \gamma = 2/3 \) for an axisymmetric unit cell defined by Chen and Butcher [192], the relation between \( \chi \) and geometrical parameters can be written as:

\[
\chi = \frac{r}{R} = \left(\frac{f}{\gamma} \vartheta\right)^{1/3} \tag{2.24a}
\]

\[
\vartheta = \frac{H}{R} = \vartheta_0 \exp\left(\frac{1}{\gamma} \varepsilon_{eq}^p\right) \tag{2.24b}
\]

\[
\vartheta_0 = \frac{H_0}{R_0} \tag{2.24c}
\]

where \( \vartheta \) and \( \vartheta_0 \) are the current and initial void distribution parameter, respectively.

Benzerga [203, 206, 207] extended the Thomason’s plastic limit load coalescence criterion for different void shapes from needle to penny shape void for different triaxialities, especially low stress triaxialities. However, no microshear localization or material properties are considered in his model.

\[
\frac{\sigma_I}{\sigma_{eq}} = \alpha \left(\frac{\chi^{-1} - 1}{W^2 + 0.1 \chi^{-1} + 0.02 \chi^{-2}}\right)^2 + \frac{\beta}{\sqrt{\chi}} \left(1 - \pi \chi^2\right) \tag{2.25a}
\]

\[
\alpha = 0.1 \quad \text{and} \quad \beta = 1.3 \tag{2.25b}
\]

Gammage et al. [208] proposed his micro-crack linkage model based on Thomason’s coalescence criterion in the intervoid ligament for a penny shaped crack in metal matrix composites. Based on Gammage’s model, the coalescence occurs when the far field work hardening rate \( \theta \) becomes equal to the stress acting between two penny shaped cracks separated by a distance \( \lambda \):

\[
\theta = \sigma_a \left[1 + \alpha \sqrt{\frac{a}{\lambda}}\right] \tag{2.26}
\]
where \( a \) is the average particle diameter, considered as an assumption or an experimental value [209]; \( \alpha \) is a stress concentration factor in the order of 2 and \( \sigma_a \) represents the far field applied stress of the participating phase. It showed good agreement with experiment for the coalescence of penny shaped voids formed by particle cracking in a metal matrix composite.

### 2.8 Post-coalescence regime

When the void volume fraction in the material reaches a critical value \( (f_c) \), coalescence begins and the load-bearing capacity of the material starts to decrease rapidly. As the void volume fraction continues to increase, it reaches the critical value \( (f_F) \) when final fracture or complete failure occurs [61]. Having derived the critical void volume fraction at coalescence using the coalescence criterion, the effective void volume fraction \( (f^*) \) can be defined by a void growth acceleration function, which is given by:

\[
f^* = \begin{cases} 
  f & \text{if } f \leq f_c \\
  f_c + \delta (f - f_c) & \text{if } f \geq f_c
\end{cases} \tag{2.27a}
\]

\[
\delta = \frac{f_u^* - f_c}{f_F - f_c} \tag{2.27b}
\]

where \( \delta \) and \( f_u^* \) are the phenomenological multiplicative void growth acceleration factor and final effective void volume fraction when \( f = f_F \), where the load bearing capacity decreases to zero, respectively [106, 107].

### 2.9 Summary

Due to the composite microstructure of dual phase steels, which consist of ferrite, martensite and sometimes bainite, and the heterogeneous distribution of microstructural features such as martensite bands and ferrite grain size, damage models, complementary functions and criteria should be accurately configured. The first step is
to choose and fit a suitable strain-, strain rate- or temperature-dependent hardening model to the hardening flow curve of the material obtained from the experiments. The next step is to determine an appropriate and applicable constitutive damage model. Phenomenological damage models, such as JC model, MMS and GISSMO are calibrated by mechanical tests and the damage evolution is evaluated by means of a linear or non-linear damage accumulation parameter. As this parameter increases, the load carrying capacity of the material decreases continuously until the final failure. On the other hand, micromechanical damage models, such as the Rice-Tracey, GTN and Rousselier models are established based on the evolution of the average void volume fraction. The material fails when the void volume fraction reaches a critical value. These models should accompany other complementary functions and criteria such as stress or strain controlled void nucleation functions and a coalescence criterion in order to predict damage evolution and material response accurately. These models, functions and criteria should be calibrated based on mechanical tests and microstructural investigations.

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Material model framework

3.1 An introduction to cellular automata

Cellular automata (CA) is a useful model for the study of dynamic or non-equilibrium or heterogeneous systems especially when processes with different natures, such as chemical, physical and metallurgical, are involved \[1\] \[2\]. CA provides a large class of frameworks for a variety of discrete, homogeneous or heterogeneous models with homogeneous interactions. \[2\]. Cellular automata, as a methodology, was first proposed by von Neumann \[3\] and then developed by Wolfram \[4\] \[5\] to simulate time-dependent space-evolving dynamic systems.

The basic steps to describe a CA modelling procedure can be written as follows \[6\] \[7\]:

1. the 3D- or 2D-space in which the model is established, should be partitioned into discrete cells (usually a cubic or square lattice) with a finite volume.

2. usually two or more cell states are assigned to each cell. Also, each cell may contain some properties associated with the investigated material or space.

3. at each time step, the neighbouring cells in the vicinity of a cell should be identified. Different approaches can be used for defining the neighbouring cells such as von Neumann, Moore or extended Moore, as shown in \[3.1\].
4. the switching or transfer rule is defined based on global deterministic or probabilistic transformation rules that change each cell state from one to another based on the properties and the current states of its neighbouring cells.

5. the transfer rule is used to update the state variable of a cell at the end of the CA cycle. This new state is used as the basis of the next cycle for the next time step. The CA model continues to iterate until a certain criterion is ultimately satisfied or for a predefined period of time.

Figure 3.2 summarizes a typical CA modelling cycle.

Figure 3.1: Different approaches for identifying neighbouring cells [8, 9]

Figure 3.2: The schematic steps of describing a CA model
The concept of CA has been extensively used by various researchers and materials scientists to simulate different metallurgical and materials related phenomena. Doherty et al. [10] and Rollett [11] reviewed the application of different computational models, including CA, to investigate recrystallization phenomena. Liu et al. [12] were among the first researchers to employ CA in order to model the curvature driven grain growth process. Li et al. [13, 14] published a study of the growth modes of individual ferrite grains in the austenite to ferrite transformation of low carbon steels using a combination of CA and Monte Carlo methods. Janssens [6] presented some advanced concepts employed by CA method to simulate the motion of grain boundaries in evolving microstructures. Cellular automata was widely used by Raabe to model and simulate the restoration phenomena, i.e. static and dynamic recrystallization [8, 15, 16]. Also, It has been used to model dendrite solidification and growth in Al-Cu alloys [17] and in hexagonal crystals [18].

However, the combination of CA and FE, shown in Fig. 3.3 has been utilized for grain refinement and solidification [19], primary static recrystallization [20], and modelling of oxide scale failure [21]. Beynon et al. [22] were the first researchers to employ CA+FE in order to model forming and damage behaviour of materials. After that, Shterenlikht used it to simulate ductile and brittle fracture and the transient temperature in thermo-mechanically controlled rolled (TMCR) steels and cleavage propagation across crystal boundaries in polycrystalline microstructures [23–25] and Perzynski et al. [26, 27] utilized it to model the failure in multi-phase materials. This model has also been used to evaluate the microstructural response in the cracking of the oxide scale and in dynamic recrystallization during the hot working of steel [28, 29], to predict grain size distribution during friction stir welding (FSW) of aluminium blanks [30], predict dynamic strain induced transformation [31], and to simulate hot deformation of aluminium alloys [32].
3.2 Hybrid model description

The structure and details of the hybrid FE-CA framework used in this work, was presented in detail by Shterenlikht [23] and the implementation somehow follows the integration procedure developed by Shterenlikht [23]. Unlike the conventional FE analysis method where the elements are both structural and material units at the same time, the elements in the FE model are responsible to determine the macro-scale strain and stress states and damage variables throughout the deformable body, and cells are employed to represent microstructural properties and evaluate the damage evolution. Das et al. [28] described four fundamental steps to create a FE-CA model:

1. define one or more arrays of cells to represent relevant micro-scale or meso-scale structural properties or features

2. identify a transfer function which allows the state of a cell to change at each increment of deformation

3. scattering step, in which significant macroscopic field variables, derived at each FE Gauss point, are distributed throughout the CA model (i.e. to the cells of the associated CA array)

4. gathering step, in which the response of the CA array is gathered and rules are set to communicate between cell arrays and the corresponding FE Gauss point through appropriate field or state variables
In this model, two 3D-cubic cell arrays are used to partition the space for each Gauss point; one array representing the ductile damage behaviour and the other representing the brittle fracture mechanism. The total number of cells in each array can be calculated based on the number of brittle cells per linear FE \( c_d \) and \( c_b \) for ductile and brittle CA, i.e. total number of cells in the ductile and brittle cell arrays are \( D_d = c_d^3 \) and \( D_b = c_b^3 \) respectively. Similar to Shterenlikht’s work \[23\], the cells in both cell arrays are neither deformable nor time-dependent. The cell sizes in the ductile and brittle arrays are independent of each other but depend on the micromechanical size scale, as described by Xia et al. \[33\] and Faleskog et al. \[34\] who introduced the concept of “damage cell” or “computational cell”. The damage cell size for ductile and brittle fracture is reported to be 0.1-0.5 mm and 0.005-0.05 mm (or 10 – 20 times larger than the median grain size), respectively \[23,35\]. These sizes are related to the observed cleavage facet size, and the spacing between large voids on the fractured surface \[24,36\]. Due to the nature of brittle mode of fracture, its damage cell size should be significantly smaller than that of ductile damage mode. At three-dimensional 26-cell Moore neighbourhood was used for each individual cell. The properties, i.e. the direction cosines of each neighbouring cell relative to the central cell, the cell coordinates as well as cell numbers, are given in Fig. 3.4.
In a CA array, each cell, regardless of the array size and position of the cell, should have a 26-cell neighbourhood. This implies the concept of “self-closing boundary condition” which means that for a cell lying at the edge of a CA the corresponding cells of the opposite edge are considered adjacent. Therefore, for a cell on the edge of a CA array, its 26 neighbouring cells are located at the opposite edges, as shown in Fig. 3.5.
For each ductile or brittle cell array, two under-structural arrays with the same size must be defined containing associated cell properties \( N = 1 \ldots n \) such that \( n \) is the total number of properties of each cell) and state variables \( Q = 1 \ldots q \) such that \( q \) is the total number of state variables defined at each CA cell). It is worth noting that to assign the properties of each cell in either a ductile or brittle CA array, a sophisticated random number generator, which is a combination of subtractive Fibonacci generator with a Marsaglia shift sequence along with an additional (different) Marsaglia shift sequence is employed to ensure that perfectly random numbers are generated [37]. Either a uniform, normal or Weibull distribution function can be selected to be used along with the random number generator.

### 3.2.1 Ductile cell array

In this research, a modified Rousselier damage model [38, 39] was employed to evaluate the ductile damage behaviour of a dual phase (DP) steel in the ductile cell array. The total number of cells in a CA array should be chosen with respect to the ductile
damage cell size. Therefore, the relation between the total number of ductile cells in a FE \( (D_d) \) and the size of the FE is given by:

\[
L_d = \sqrt[3]{\frac{L_i \times L_j \times L_k}{D_d}} \tag{3.1}
\]

where \( L_i, L_j \) and \( L_k \) are the size of the FE in each direction and \( L_d \) denotes the ductile damage cell size. For each cell, only one property is assigned which is the critical Rousselier damage variable at failure \( (\beta_F) \) based on the initial volume fraction of the material \( (\Xi_{m(d)}^1) = f_0 \). A normal distribution random number generator is used to generate \( f_0 \) in each cell at the beginning of the simulation. The only state variable in each cell is the current value of the scalar damage variable \( (\Phi_{m(d)}^1(t_i) = \beta_{m(t_i)}) \). Each ductile cell \( m \) can take one of two possible states according to the following criterion:

\[
S_{m(d)}(t_{i+1}) = \begin{cases} 
\text{alive} & \quad \text{if} \quad \beta_{m(t_{i+1})} < \beta_F \\
\text{dead} & \quad \text{if} \quad \beta_{m(t_{i+1})} \geq \beta_F 
\end{cases} \tag{3.2}
\]

\[
S_{m(d)}(t_{0}) = \text{alive}
\]

### 3.2.2 Brittle cell array

Similar to ductile cell arrays, the relation between the total number of brittle cells in a FE \( (D_b) \) and the size of the FE is written by:

\[
L_b = \sqrt[3]{\frac{L_i \times L_j \times L_k}{D_b}} \tag{3.3}
\]

where \( L_b \) represents the brittle damage cell size. The brittle cell size should be chosen based on the matrix grain size for a progressive brittle grain-to-grain fracture model. Each cell \( m \) in the brittle CA array carries two different properties: (1) fracture stress \( (\Xi_{m(b)}^1) = \sigma_{m}^F \) calculated based on a Weibull distribution random number generator assigning a grain size value to each cell, and (2) grain orientation \( (\Xi_{m(b)}^2) = \alpha^m \) obtained by a uniform distribution random number generator, in order to simplify.
the model and reduce computational cost. Although the grain orientation is usually defined by two angles, the grain was described by a single orientation angle provided by a uniform distribution random number generator. Accordingly, the difference between grain orientation type of cell \(m\) and its neighbouring cell \(l\) is calculated via \(|\alpha^m - \alpha^l|\). Thus, this can be considered similar to the actual grain misorientation angle. This was used in this model to determine whether or not the crack growth can be inhibited or arrested by a high-angle misorientation grain boundary \([40, 41]\). A crack can grow from a cell \(m\) in the brittle cell array to another cell \(l\) in its vicinity if the absolute value of the difference between their orientations is less than a critical misorientation threshold \((\alpha_c)\) which is considered to be a material property.

The main mechanism for the initiation of brittle fracture initiation in DP steels is martensite cracking. A brittle crack initiates perpendicular to the tensile stress. To include this mechanism in the model, at the beginning of the simulation, the volume fraction of martensite should be introduced into the model as a material property and different kinds of distribution functions can be used to assign a special state to particular cells: \(alive_m\) or “alive with martensite” which can be considered as a potential site for brittle crack initiation. Only these cells can take part in crack initiation. The state of other cells would be “alive” at the beginning of the simulation. Cells in the brittle CA array can fail due to brittle fracture criterion \((dead_b)\) when the maximum principal stress \((\sigma_{m}^i(t_i))\) exceeds the fracture stress defined for that particular cell. It becomes dead due to the synchronization or mapping technique with ductile cell array which reflects dead cells as a result of ductile fracture \((dead_d)\). Therefore, each brittle cell can take one of four possible states: \(alive, alive_m, dead_b\) and \(dead_d\). The state of each cell in the brittle CA array is determined by the following.
criterion:

\[
S_m(t_{i+1}) = \begin{cases} 
\text{dead}_b & \text{if } ( [S_{m(b)}^l(t_i) = \text{dead}_b \lor S_{m(b)}^m(t_i) = \text{dead}_d ] \land \{ \sigma^m_F(t_i) \geq \sigma^m_F \land \{ S_{m(b)}(t_i) = \text{alive}_m \} \lor \} \land \\
\text{alive}_m & U = 1 \ldots u \\
\text{alive} & V = 1 \ldots v \\
\end{cases}
\]

\[u + v = D_b\]  

(3.4)

where \(S_{U(b)}, S_{V(b)}, u\) and \(v\) are the state and total number of cells with and without martensite, respectively.

### 3.2.3 Transfer rule

An important step in defining a CA model is to set a time-dependent transfer function to update cell state in each time increment. The general transfer rule function in this model is given by:

\[
S_m(t_{i+1}) = \Omega \left( S_m(t_i), S_{m}^l(t_i), \Xi^N_m, \Xi^N_l, \Phi^Q_m(t_i) \right) \]

(3.5)

which means that the new state of each cell \(m\) is a function of its current state \((S_m(t_i))\), the current state of its neighbouring cells \((S_{m}^l(t_i))\), its properties \((\Xi^N_m, N = 1 \ldots n)\), the properties of its neighbouring cells \((\Xi^N_l, N = 1 \ldots n)\), and the state variable of cell \(m\) at the time \(t_i\) \((\Phi^Q_m(t_i), Q = 1 \ldots q)\). Cell properties are intrinsic material properties and the state variables are determined from the solution of the constitutive material model. In this model, two CA arrays, ductile and brittle CA arrays, are used to evaluate two modes of fracture. They follow rules and criteria that are independent of each other, however, since these two arrays represent the same physical space, the state of cell \(m\) in one array would be dependent on the state of a group of cells \(g\) in
the other array. It means that if a cell status changes from \textit{alive} to \textit{dead} in either the ductile or brittle CA array, it should be reflected in the other array in order to take the loss of integrity into account for both CA arrays. Accordingly, the full transfer rule for both ductile and brittle CA arrays can be written as:

$$S_{m(d)}(t_{i+1}) = \Omega_d \left( S_{m(d)}(t_i), S_{m(d)}^l(t_i), \Xi_{m(d)}^N, \Xi_i^N, \Phi_{m(d)}^Q(t_i), S_{g(b)}(t_{i+1}) \right)$$

(3.6a)

$$S_{m(b)}(t_{i+1}) = \Omega_b \left( S_{m(b)}(t_i), S_{m(b)}^l(t_i), \Xi_{m(b)}^N, \Xi_i^N, \Phi_{m(b)}^Q(t_i), S_{g(d)}(t_{i+1}) \right)$$

(3.6b)

where subscripts \(d\) and \(b\) refer to the ductile and brittle cell arrays, respectively. The number of cells \(g\) depends on the total number of cells in each CA array \((D_d \text{ and } D_b)\).

The link between CA arrays and FE is established through solution-dependent state variables \((R^i_p)\) for each finite element integration point \(i\), as shown in Eq. 3.7:

$$R^i_p(t_{i+1}) = \Psi(S_{m(d)}(t_{i+1}), S_{m(b)}(t_{i+1}))$$

(3.7)

where \(R^i_p(t_{i+1})\) is the updated state variable \(P (P = 1 \ldots p)\) at time \(t_{i+1}\) for integration point \(i\). For each integration point, three solution-dependent variables are defined based on the states of the brittle and ductile CA cells. The number of brittle cells due to the brittle and ductile fracture modes and total number of dead brittle and ductile
cells are calculated via Eq. 3.8a, Eq. 3.8b, Eq. 3.8c and Eq. 3.8d respectively.

\[
X^b_{(b)}(t_i) = \sum_{m=1}^{D_b} \forall m : S_{m(b)}(t_i) = \text{dead}_b
\]  
(3.8a)

\[
X^d_{(b)}(t_i) = \sum_{m=1}^{D_b} \forall m : S_{m(b)}(t_i) = \text{dead}_d
\]  
(3.8b)

\[
X_{(b)}(t_i) = X^b_{(b)}(t_i) + X^d_{(b)}(t_i)
\]  
(3.8c)

\[
X_{(d)}(t_i) = \sum_{m=1}^{D_d} \forall m : S_{m(d)}(t_i) = \text{dead}
\]  
(3.8d)

Subsequently, three FE solution-dependent variables are written as:

\[
R_1(t_i) = \frac{X^b_{(b)}(t_i)}{X_{(b)}(t_i)}
\]  
(3.9a)

\[
R_2(t_i) = 1 - \frac{X_{(d)}(t_i)}{X_{max}^{(d)}} - \frac{X^b_{(b)}(t_i)}{X_{max}^{(b)}}
\]  
(3.9b)

\[
R_3(t_i) = \begin{cases} 
\text{dead} & \text{if } R_2(t_i) \leq 0 \\
\text{alive} & \text{otherwise}
\end{cases}
\]  
(3.9c)

where \(X_{max}^{(d)}\) and \(X_{max}^{(b)}\) are the maximum number of dead cells allowed in the ductile and brittle cell arrays, respectively. As described by Shterenlikht [23], if the number of dead cells reaches its maximum limit, then a crack or void coalescence takes place and the FE would lose all its load-bearing capacity and should be removed from the model. In Eq. 3.9a-3.9c, \(R_1(t_i)\) represents the fraction of brittle fracture and is between \([0\ldots1]\), such that 0 means no brittle fracture and 1 means 100\% of failure mode is due to brittle fracture mode; \(R_2(t_i)\) is called integrity and \(R_2 \in [-1\ldots1]\), and \(R_3(t_i)\) denotes the state of the finite element. The initial values of the solution-dependent
variables for each FE are:

\[
\begin{align*}
R_1(t_0) &= 0 \\
R_2(t_0) &= 1 \\
R_3(t_0) &= \text{alive}
\end{align*}
\] (3.10)

### 3.2.4 The model cycle

At each time increment, the following steps are performed for each FE at the corresponding ductile and brittle CA arrays. It is worth noting that the FEs are responsible for capturing the constitutive response of the material subjected to deformation and the CA arrays are used to determine the damage and fracture behaviour [23].

1. At each integration point, the Cauchy stress tensor \((\sigma_{ij})\) and strain tensor \((\varepsilon_{ij})\) are calculated via the constitutive material model and the integration procedure of the Rousselier damage model.

2. The value of the Rousselier scalar damage variable \((\beta)\) is determined. In addition, the maximum principal stress \((\sigma_I)\) and its corresponding direction cosines \((d_k)\) are calculated.

3. The damage variable at each cell \(m\) in the ductile cell array at the time \(t_{i+1}\) is determined using the following criterion:

\[
\forall m : \beta_m(t_{i+1}) = \beta(t_{i+1}) \tag{3.11a}
\]

\[
\forall S_{m(d)}(t_i) = \text{dead} \quad \text{if} \quad d_k^m.d_k(t_i) \simeq 1 \implies \beta_l(t_{i+1}) = C_D \cdot \beta(t_{i+1}) \tag{3.11b}
\]

where \(C_D\) is the damage concentration factor for ductile cell array and \(d_k^m\) are the direction cosines of the line connecting the centres of cells \(m\) and \(l\).

4. The state of each cell in the ductile CA array \((S_{m(d)}(t_{i+1}))\) is obtained according to Eq. 3.2.
5. All dead cells in the ductile CA array should be reflected to the brittle cell array with a mapping function. This function distributes the array of ductile cell states across the brittle cell array and the result is called synchronization array of brittle cell states ($S_{m(bd)}(t_{i+1})$).

$$S_{m(bd)}(t_{i+1}) = M_{d\rightarrow b}(S_{m(d)}(t_{i+1})) \quad (3.12a)$$

The $\bar{m}$ denotes the corresponding cells in the brittle CA array. The mapping rule can be written as:

$$S_{m(b)}(t_{i+1}) = \begin{cases} 
\text{dead}_d & \text{if } S_{m(bd)}(t_{i+1}) = \text{dead} \land \left( S_{m(b)}(t_i) = \text{alive} \lor S_{m(b)}(t_i) = \text{alive}_m \right) \\
S_{m(b)}(t_i) & \text{otherwise}
\end{cases} \quad (3.12b)$$

6. Similar to step 3, the maximum principal stress in each cell in the brittle CA array is calculated using the following criteria:

$$\forall m : \sigma^m_I(t_i) = \sigma_I(t_i) \quad (3.13a)$$

$$\forall S_{m(b)}(t_i) = \text{dead}_b \text{ if } d^b_k(t_i) \simeq 1 \implies \sigma^I_I(t_i) = C_B \cdot \sigma_I(t_i) \quad (3.13b)$$

$$\forall S_{m(b)}(t_i) = \text{dead}_d \text{ if } d^b_k(t_i) \simeq 1 \implies \sigma^I_I(t_i) = C_D \cdot \sigma_I(t_i) \quad (3.13c)$$

7. Similar to step 4, the state of each cell in the brittle cell array ($S_{m(b)}(t_{i+1})$) is determined using Eq. 3.4.

8. Like step 5, all dead cells in the brittle cell array should be reflected in the ductile cell array via the mapping function to build the synchronization array of ductile cell states ($S_{m(db)}(t_{i+1})$).

$$S_{m(db)}(t_{i+1}) = M_{b\rightarrow d}(S_{\bar{m}(b)}(t_{i+1})) \quad (3.14a)$$
\[ S_{m(b)}(t_{i+1}) = \begin{cases} 
\text{dead} & \text{if } S_{m(db)}(t_{i+1}) = \text{dead} \land S_{m(d)}(t_{i}) = \text{alive} \\
S_{m(b)}(t_{i}) & \text{otherwise}
\end{cases} \]

The application of the mapping function is illustrated in Fig. 3.6 for both \( M_{d\rightarrow b}(S_{m(d)}(t_{i+1})) \) and \( M_{b\rightarrow d}(S_{m(b)}(t_{i+1})) \).

Figure 3.6: Illustration of the mapping operation

9. In this step, the FE solution-dependent variables \( R_k(t_i), k = 1, 2, 3 \) are calculated for each integration point based on Eq. 3.9a-3.9c.

10. Calculated solution-dependent variables are returned to ABAQUS/Explicit solver for the next time increment.

Figure 3.7 shows a schematic chart of the sequence of operations performed at each time increment for each FE and the corresponding two CA arrays of the model.
• Perform the transfer rule
• Determine the new state of each cell
• Calculating solution dependent variables
• Obtaining state of CAs and FEs

• Calculating stress and strain tensor
• Calculating damage variable

Start

Abaqus solver
Material model
Array and element status
Cellular automata arrays

Finite element
CA array

Dead Finite element (no load bearing capacity)
Dead array

Active Finite element
Active array

Finite element
CA array

Figure 3.7: Sequence of steps performed in the model for each FE integration point and corresponding CA arrays

3.3 Bibliography


Chapter 4

Effect of rate-dependent constitutive equations on the tensile flow behaviour of DP600 using Rousselier damage model

In this chapter, the Rousselier ductile damage model was employed to model hardening, plastic instability and damage properties of DP600 during uniaxial tension in a wide range of strain rates (from 0.001 to 1000 s\(^{-1}\)). Also, various well-known phenomenological hardening functions, such as Johnson-Cook and KHL as well as a modified version of Johnson-Cook and multiplicative combinations of Voce with other strain-rate hardening functions have been fitted to experimental flow curves via a new combination of non-linear regression and Markov chain Monte Carlo (MCMC) method. The effect of each hardening function on the evolution of the damage parameter, void volume fraction and strain distribution along the gauge length was evaluated throughout the deformation. Also, the onset of instability, geometry of the neck and final fracture were then assessed by comparing the numerical results with experimental data. It is found that the modified JC and Voce-modified JC models can predict the flow behaviour of DP600 more accurately. Additionally, it is shown that the strain hardening rate at large strain levels, as determined by the hardening models, has a considerable effect on the strain map along the specimen, onset of void growth, and
progression of damage in the localized area.

4.1 Introduction

There is an increasing demand in the automotive industry to reduce both vehicle weight and gas emissions, and to increase fuel efficiency. Therefore, significant effort has been invested to develop suitable materials which can exhibit improved performance in terms of combined high ductility, formability and strength [1, 2]. Advanced high strength steels (AHSS), such as dual phase (DP) steels, offer high strength-to-weight ratio and improved crash resistance [3]. Dual phase steels, being low carbon steels, belong to a family of high strength strip grades which consist of hard second phase islands (usually martensite) distributed across a ductile ferritic matrix. To obtain such a microstructure, dual phase steels are annealed by holding a strip in the ferrite-austenite temperature region for a period of time, followed by controlled quenching so that austenite transforms to soft ferrite and hard martensite [4, 5]. Dual phase steels show low yield strength and high ultimate tensile strength, which result in high strain hardenability. They also exhibit continuous yielding behaviour, high strain hardening rates at low strain values and large uniform elongation [3, 6].

Due to the growing application of DP steels in the automotive sheet metal forming industry, accurate prediction of their deformation behaviour and formability is essential for manufacturers to produce defect-free components. Usually, conventional strain-rate processes such as stamping, drawing or hydroforming are used to manufacture auto-parts [7, 8]. However, high strain-rate forming techniques based on explosive forming (EF) and electro-hydraulic forming (EHF), which can increase formability and uniformity of strain [9, 10], are also generating great interest in the automotive industry. Thus, accurate prediction of forming behaviour, from quasi-static to high strain rates is necessary to reduce the cost and time needed for successful part fabrication [11, 12]. In this regard, various phenomenological and micromechanical models, have been developed for finite element analysis to predict component formability and failure of DP600 sheets during cross-die test [12, tube hydroforming [13], tube hydropiercing [14], and electrohydraulic free-forming and die-forming [9, 10]. It has been shown
by several researchers that the predominant damage mechanism and failure in DP steels depends on the ferrite and martensite grain sizes and their morphology [15] [17], and can range from a mixture of brittle and ductile rupture to completely ductile rupture in a quasi–static uniaxial tension test. The main mechanisms of ductile failure generally consist of nucleation, growth and coalescence of voids during the forming process [16, 17], although the fracture mechanism can vary from a shear mechanism at negative stress triaxialities to a combination of shear and void formation at low triaxialities [18]. Therefore, micromechanical damage models which account for these mechanisms are more suitable to numerically evaluate ductile failure in metal forming simulations, although it is shown that it is hard to define a damage model that can predict the ductile fracture for different triaxiality levels [19].

Among micromechanical damage theories, the Gurson–Tvergaard–Needleman [20] [21] and Rousselier [22] models are two of the most widely known for modelling ductile fracture. Two main advantages of the latter is that it requires the specification of fewer parameters and it can predict the evolution of damage and consequent void volume fraction growth in pure shear deformation [23]. However, the Rousselier damage model requires an appropriate hardening equation that can predict the flow behaviour of the sheet material at different strain rates. There are many hardening constitutive models in the literature which fit quite well to the experimental data at low strain values up to uniform elongation in uniaxial tension. However, the extrapolation of flow curves beyond the range of experimental data can lead to very different results depending on the model employed [24].

The main objective of this research is two-fold. First, different phenomenological strain–rate sensitive hardening equations have been fitted to the experimental data, obtained from uniaxial tensile tests at quasi-static, medium and high strain rates, to define the hardening behaviour of DP600 sheet. A new approach based on the combination of non-linear regression (NLR) and Markov chain Monte Carlo method (MCMC) has been utilized to calculate the constants in each hardening constitutive equation. In addition to well-known hardening constitutive functions, multiplicative combinations of Voce [25] strain hardening, and three strain–rate functions have been used. The accuracy of these different functions is evaluated via widely-accepted
statistical criteria, the root-mean-square error (RMSE) and the so-called adjusted R-squared value. Secondly, the mechanical response, onset and evolution of strain localization and failure, the geometry of the instability as well as the evolution of void volume fraction are investigated using the Rousselier damage model implemented in a user material subroutine (VUMAT) that is used in ABAQUS/Explicit FE simulation software. The effect of different hardening functions on the mentioned parameters, and their advantages and drawbacks will be discussed.

4.2 Constitutive modelling

4.2.1 Rousselier damage model

The Rousselier model [22] is a thermodynamically consistent damage model which uses the ‘simplest assumption’ at each stage of its development [26]. It is an elastic-plastic constitutive law that employs cumulative plastic strain ($p$) and cumulative damage variable ($\beta$) which corresponds to the void volume fraction to model the ductile damage and rupture behaviour of porous materials [27, 28]. It describes the increase in void volume fraction in a ductile domain with isotropic hardening and isotropic damage [29]. The Rousselier plastic potential is given by:

$$\varphi = \sigma_{eq} - H + B(\beta)D \exp \left( \frac{\sigma_m}{(1 - f)\sigma_I} \right) = 0 \tag{4.1}$$

in which $\sigma_{eq}$ is the von Mises equivalent stress (such that $\sigma_{eq} = (\frac{3}{2}S_{ij}S_{ij})^{1/2}$ where $S_{ij}$ is the deviatoric stress) and $\sigma_m$ is the hydrostatic stress (such that $\sigma_m = \frac{1}{3}tr(\sigma_{ij})$ where $\sigma_{ij}$ is the Cauchy stress). $D$ and $\sigma_I$ are material parameters which describe the resistance of the material to void growth and coalescence [23, 29]. $H$ is the hardening curve of the material; $B(\beta)$, the damage function, is the conjugate force to damage parameter $\beta$, $f_0$ and $f$ are the initial and current void volume fraction, respectively. The damage variable $\beta$ and $f$ are directly related to the plastic multiplier in the normality rule ($\lambda$) and follow the strain increment ($\dot{p}$) and increase with the deformation:
\[
\dot{f} = (1 - f) \dot{p} f D \exp \left( \frac{\sigma_m}{(1 - f)\sigma_I} \right)
\]

\[
\dot{\beta} = \dot{p} D \exp \left( \frac{\sigma_m}{(1 - f)\sigma_I} \right)
\]

(4.1a)

(4.1b)

The relation between current void volume fraction and \(B\) is given by:

\[
f = \frac{B(\beta)}{\sigma_I} = \frac{f_0 \exp(\beta)}{1 - f_0 + f_0 \exp(\beta)}
\]

(4.1c)

Li et al. [26] presented an explicit and detailed theoretical calculation procedure of the Rousselier damage model and its related parameters. In the original Rousselier model, void nucleation was not considered and failure was described by specifying a critical void volume fraction \((f_c)\) which corresponds with a critical value of the damage parameter \(\beta_c\). Along the deformation process, material hardening (described by the second term of Eq. 4.1) is overtaken by the material softening (third term of Eq. 4.1) due to the increase in \(f\) to a critical level beyond which the material completely loses its load–bearing capacity and faces local failure [29, 30].

4.2.2 Hardening constitutive models

In the simulation of metal forming processes, hardening and softening of the sheet material are dependent on thermomechanical parameters derived from experimental flow curves. Therefore, it is important to carefully determine the parameters in a hardening equation, whether it is a phenomenological, physically–based or artificial neural network model [31], so that the mechanical behaviour of the sheet material can be accurately predicted. Since ductile metals and alloys can be safely deformed up to high strain values, the formulation of these equations in terms of predicting hardening behaviour and hardening rate is critical [24, 32]. Therefore, in this study, different phenomenological plastic hardening equations have been used to identify the effect of hardening functions on the deformation and damage simulation of DP600 at different strain rate levels. Although most of these phenomenological hardening models can be described based on plastic strain, deformation rate and forming temperature.
\( H = \sigma(\varepsilon_p, \dot{\varepsilon}_p, T) \), no parameter was calculated for the temperature-dependent part of the function since the experimental tests were carried out at ambient temperature and the temperature rise due to adiabatic heating was shown to be negligible for the investigated range of strain rates \[8\]. In the following functions, \( C_1, C_2, \ldots, C_n \) are materials constants which can be determined by an appropriate fitting procedure and \( H, \varepsilon_p, \dot{\varepsilon}_p \) denote the matrix flow stress, the equivalent plastic strain, the equivalent plastic strain rate, respectively.

The isotropic non-linear hardening behaviour of materials can be described by a power hardening law. This form of power law \[33\] has been extensively used in the literature \[34–36\] and is written as

\[
H = C_1 \left( \frac{\varepsilon_p}{C_1} E + 1 \right)^{C_2} \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_3} \quad (4.2)
\]

where \( E \) is Young’s modulus \((E=210 \text{ GPa for DP600}[37])\) and \( \dot{\varepsilon}_0 \) represents a reference strain rate.

The Johnson-Cook (JC) model is one of the most widely-used hardening equations to describe the flow stress at different strain rates and temperatures \[38\]. The original form of the JC model is given by:

\[
H = (C_1 + C_2 \varepsilon_p^{C_3}) \left[ 1 + C_4 \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right) \right] \quad (4.3)
\]

Previously, various researchers have calculated the parameters in the JC model for DP steels, such as DP500 \[39\], DP590 \[10\], DP780 \[40\], and DP1200 and DP1400 \[41\], while others modified the JC model, mostly by considering the effect of temperature on the hardening behaviour \[31, 42\]. Holmquist and Johnson \[43\] indicated that the effect of strain rate on the material strength cannot be described accurately by a linear function of natural log as represented in the JC model, and it is necessary to modify the strain rate hardening term to model this behaviour. In this study, a simple modification, as can be seen in Eq. \[4.4\], was incorporated in the JC hardening model so that the flow curves of DP600 at different strain rates can be modelled more
precisely. The modified-JC model (mJC) is given by:

$$H = \left( C_1 + C_2 \varepsilon_p^C \right) \left[ 1 + C_4 \left( \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \right]$$  (4.4)

One of the most important saturation–type strain hardening functions was proposed by Voce \[25\] in which the strength of the material reaches a saturation point (\(\sigma_s\)) and remains constant, i.e. the strain hardening rate reduces to zero beyond a certain strain level. It is worth noting that the original Voce function did not include a strain-rate or temperature dependent part. Accordingly, different linearly combined functions based on Voce, as the strain hardening part, and other strain-rate and temperature sensitive functions have been proposed in the literature for DP steels, such as DP590–DP780–DP980 \[44\], DP800 \[45\] and DP600 \[8\], and TRIP steels \[46\]. Since the Voce model can successfully describe the flow behaviour of many sheet materials, the strain–dependent Voce equation (Eq. 4.5b) was combined with three strain–rate dependent functions, by multiplying the Voce equation with (1) a power-law (Eq. 4.5c), (2) strain rate term of the Johnson-Cook model (Eq. 4.5d), and (3) strain rate term of the modified Johnson-Cook function (Eq. 4.5e). All three multiplicative combinations were evaluated to determine which one more accurately describes the flow curve of DP600 at different strain rates.

$$H = f(\varepsilon_p) g(\dot{\varepsilon}_p)$$  (4.5a)

$$f(\varepsilon_p) = C_1 - (C_1 - C_2)(1 - \exp(-C_3 \varepsilon_p))$$  (4.5b)

$$g(\dot{\varepsilon}_p) = \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_4}$$  (4.5c)

$$g(\dot{\varepsilon}_p) = \left[ 1 + C_4 \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right) \right]$$  (4.5d)

$$g(\dot{\varepsilon}_p) = \left[ 1 + C_4 \left( \ln \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \right]$$  (4.5e)

The Khan–Huang–Liang (KHL) \[47\] model (Eq. 4.6) is a constitutive model in which the stress is unbounded at large strains \[44\] \[48\]. The KHL model is able to capture the hardening response of engineering materials such as advanced high strength steels
(AHSS) [49], aluminium alloys [50] and titanium alloys [48] [51] over a wide range of strains and strain rates:

\[
H = \left[ \frac{C_1}{C_2} + \left( 1 - \frac{\ln \dot{\varepsilon}_p}{\ln D_0^{p}} \right) C_4 \frac{\dot{\varepsilon}_p}{\varepsilon_p} C_5 \right] \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^C_5
\]

(4.6)

where $\dot{\varepsilon}_0$ and $D_0^p$ denote the reference strain rate and the upper bound strain rate which can be arbitrarily chosen to be $10^6 \text{s}^{-1}$ [49]. The reference strain rate was chosen as $1 \text{s}^{-1}$ for the JC, modified–JC, Voce–type functions and KHL hardening model. For some materials, the KHL model leads to a better prediction of material hardening than strictly multiplicative models and will therefore be used in this investigation.

4.3 Material and Methods

4.3.1 Material

The material used in this study was a DP600 sheet with a nominal thickness of 1.48 mm and having phase volume fractions of 92.0, 4.7 and 3.3 vol% ferrite, martensite and bainite content, respectively. The chemical composition of as-received DP600 sheet is given in Table 4.1.

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>Cr</th>
<th>Mo</th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.107</td>
<td>1.5</td>
<td>0.18</td>
<td>0.18</td>
<td>0.21</td>
<td>0.06</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Table 4.1: Chemical composition of as-received DP600 steel (wt%) [52]

4.3.2 Experimental procedures

Uniaxial tensile tests were conducted on DP600 sheet along the sheet rolling direction. ASTM (E8M-04) specimens were tested at low strain rates (0.001 and 0.1 s$^{-1}$) using an Instron 1331 servo-hydraulic testing machine with cross-head velocities of 3 and 300 mm/min and sampling rates of 1.67 and 167 Hz, respectively. A $\pm 12.5 \text{mm}$
biaxial extensometer was used to measure the axial and width strains. In order to conduct tests at intermediate strain rates (1, 10, 100 s\(^{-1}\)) and at a high strain rate of 1000 s\(^{-1}\), a miniature “dog–bone” shaped specimen was designed. To conduct the tests at intermediate strain rates, a special Hydraulic Intermediate Strain Rate (HISR) apparatus, developed at the University of Waterloo [53] was used and a tensile split Hopkinson bar (TSHB) apparatus was used to carry out high strain rate tests. Cross–head velocities of 750, 19500 and 180000 mm/min were employed to obtain strain rates of 1, 10, 100 s\(^{-1}\).

Strain measurements of intermediate and high strain rate tests were carried out using 2D digital image correlation (DIC) techniques along with virtual extensometers to measure the longitudinal and width strains, respectively. To use the DIC method, the specimens were first painted in white followed by the application of a stochastic black speckle pattern that deforms with the specimen during the test. A high–speed digital camera was used along with DIC processing software (ARAMIS from GOM and VIC-2D from Correlated Solutions) to calculate the longitudinal and width strains during the tests, from intermediate to high strain rates. For each strain rate, three to five tests were carried out to confirm the repeatability of the results. The measured tensile force was divided by the original cross–sectional area of the gauge and the engineering stress was then converted to true stress. The true (plastic) strain was directly obtained from the DIC software and the average true stress–true plastic strain curve was obtained for each strain rate. Rahmaan et al. [8] presented a detailed description of the testing procedures, specimens, tools and apparatus, measurement procedures and obtained results for these experiments. The averaged true stress–true strain curves of this DP600 steel sheet are shown in Fig. 4.1 [8]. These flow curves were used to calibrate various hardening functions for the strain range 0.002–0.14 and the strain rate range 0.001–1000 s\(^{-1}\).
4.3.3 Fitting procedure

In this study, the Markov chain Monte Carlo (MCMC)–Metropolis-Hastings (MH) algorithm [54] was utilized as an optimization method to determine the parameters for the hardening functions; introduced in section 4.2.2. This algorithm is a combination of the Monte Carlo method, which draws samples from a specified range for each parameter, and Markov chain which generates a sequence of random variables ($C_i$) in which the probability of current variables is dependent on the previous samples. Also, the Metropolis-Hastings algorithm helps the Markov chain with a candidate range for a set of variables [54]–[56]. Stochastic methods such as MCMC are preferred for noisy data such as tensile curve data generated at high strain rates. However, this algorithm can be computationally expensive since initial values and a certain initial wide range of random values should be chosen for each fitting parameter at the beginning of the procedure. For this reason, non-linear regression (NLR) was used to obtain parameter values which were used to initialize the MCMC optimization.

The proposed combination of NLR+MCMC is computationally fast and inexpensive compared to other optimization techniques because accurate initial values with much narrower ranges are used to initialize the MCMC process in the proposed fitting method and more rapidly lead to a precise determination of model parameters [57].
Another advantage of this fitting procedure is that it can also be used for a certain part of a function. This is very useful when fitting a multiplicative function to a data set, e.g. \( \sigma(\varepsilon_p, \dot{\varepsilon}_p) = f(\varepsilon_p) g(\dot{\varepsilon}_p) \), so that the coefficients of the strain hardening function can be calculated using non-linear regression and then the results can be exported to MCMC to determine strain-rate hardening function parameters and further calibration.

The method was implemented in a Python code and a flowchart of this algorithm is shown in Fig. 4.2. First, NLR method was performed to calculate the fitting parameters \( (C_{1...m}(t_0)) \) and their corresponding error \( (\sum_{res}(t_0)) \), based on the sum of squares of residuals, for a certain hardening equation. These values were considered as initial guess and initial error for the MCMC procedure \( (C_{1...m}^f \text{ and } \sum_{res}) \). Then a pseudo-random number generator was used to generate random fitting parameters in a narrow range \( (C_i \pm 0.2C_i) \) around the initial values \( (C_{1...m}(t_{i+1})) \) and then the least square error \( (\sum_{res}(t_{i+1})) \) was calculated and compared with the initial error. When the current error was less than the initial one, the new set of parameters was considered as the initial values and the previous error was substituted with the current least square error for the next iteration, otherwise nothing was changed and the loop continued until it reached the maximum number of iterations.
4.3.4 Finite element simulation

The Rousselier ductile damage model was implemented as a user material subroutine for use in the Abaqus/Explicit finite element software. The implementation follows the integration procedure developed by Shterenlikht [36]. The specimen geometries used for simulating the uniaxial tension tests, corresponding with the experimental specimens for quasi–static, and moderate and high strain rates are shown in Fig. 4.3a and Fig. 4.3b respectively.
To reduce computational cost, the size of the grip section was reduced compared with the actual size of the test specimens. Furthermore, only a quarter of the specimen was modelled due to the symmetries associated with the material and test geometry. The specimens were meshed using 8-node reduced integration brick elements (C3D8R in the Abaqus element library). A reference point was coupled to the top surface of the grip section (perpendicular to the y–axis) such that all degrees of freedom were constrained, except for displacement in the loading direction. The cross–head velocities corresponding to the experimental tests were applied to the reference point to obtain the same strain rates in the simulation runs. In order to calculate the stress–strain curve of the material in each testing condition, the load–displacement of this point was used to derive the flow curve and compare it with the experiments. Symmetric boundary conditions were applied to both half (x–y) symmetry planes of the specimen, i.e. the displacements were locked in the loading direction for the nodes on the symmetry plane at the centre of the gauge area, perpendicular to the specimen axis, and locked perpendicular to the loading direction for the nodes located on the model symmetry line, parallel to specimen axis.

As shown by many researchers \cite{14, 58, 59}, the damage behaviour and the slope of the non–uniform part of the flow curve are considerably mesh size–dependent. Therefore, a mesh sensitivity analysis was performed by reducing the element size from 0.5 mm to 0.1 mm for quasi-static specimens and from 0.3 mm to 0.05 mm for the higher rate specimens to determine the effect of element size on the simulation of tensile tests. Since the intermediate and high strain rate specimens are considerably smaller in size (1.75 mm wide and 1.48 mm thick) than the standard tensile specimen, it was necessary to reduce the size of the brick elements in order to maintain a uniform element aspect ratio. Simulation results showed good consistency for an element size less than 0.25 mm and 0.1 mm in the damaged area, in terms of accuracy and computational cost, for quasi-static and higher strain rate models, respectively \cite{29}. Therefore, biased meshing, ranging from 0.5 mm near the grip section to 0.25 mm near the middle of the gauge length, was used for quasi-static simulation and an element size of 0.1 mm was used for the higher rate specimens.
4.4 Results and Discussion

4.4.1 Fitting results and statistical analysis

The material parameters for the matrix flow stress equations as obtained from the MCMC optimization procedure described, can be found in Table 4.2.

Table 4.2: Coefficients of hardening functions for DP600 determined via NLR+MCMC

<table>
<thead>
<tr>
<th></th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power-law</td>
<td>318.85</td>
<td>0.1836</td>
<td>0.0151</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Johnson-Cook (JC)</td>
<td>226.99</td>
<td>846.53</td>
<td>0.3322</td>
<td>0.0166</td>
<td>-</td>
</tr>
<tr>
<td>modified JC (mJC)</td>
<td>225.35</td>
<td>850.16</td>
<td>0.3194</td>
<td>0.0037</td>
<td>1.5715</td>
</tr>
<tr>
<td>Voce-power law (VPl)</td>
<td>380.28</td>
<td>781.30</td>
<td>8.8338</td>
<td>0.0165</td>
<td>-</td>
</tr>
<tr>
<td>Voce-JC (VJC)</td>
<td>365.70</td>
<td>751.35</td>
<td>8.8338</td>
<td>0.0174</td>
<td>-</td>
</tr>
<tr>
<td>Voce-mJC (VmJC)</td>
<td>400.21</td>
<td>795.19</td>
<td>9.0236</td>
<td>0.0015</td>
<td>1.9430</td>
</tr>
<tr>
<td>KHL</td>
<td>161.54</td>
<td>946.48</td>
<td>0.2577</td>
<td>-0.1900</td>
<td>0.0037</td>
</tr>
</tbody>
</table>
Standard statistical parameters such as adjusted R-squared value (Eq. 4.7b) and RMSE (Eq. 4.7c) were employed to statistically evaluate the goodness of the fit and the accuracy of each hardening function over the entire range of strain rates. The adjusted R-squared is the modified version of R-squared value which takes the number of predictors and points into account. R-squared value increases by increasing the number of predictors whereas in adjusted R-squared value, it leads to an increase only if the new term improves the model prediction beyond what would be obtained by probability. Both the adjusted R-squared and RMSE are calculated by comparing stress values from experimental tests ($\sigma_x$) and stress values predicted by hardening models ($H$).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(\sigma_x - H)^2}{\sum_{i=1}^{n}(\sigma_x - \bar{\sigma}_x)^2}$$  \hspace{1cm} (4.7a)

$$\bar{R}^2 = R^2 - (1 - R^2)\frac{m}{n - m - 1}$$ \hspace{1cm} (4.7b)

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n}(\sigma_x - H)^2}$$ \hspace{1cm} (4.7c)

where $\bar{\sigma}_x$, $n$ and $m$ represent the mean stress value, the total number of flow curve data points and the total number of predictors ($C_{1...n}$) in the model (not counting the constant term). The results of the statistical analysis, shown in Fig. 4.4, reveal that the proposed NLR+MCMC method can improve the accuracy of the predicted flow curves by 10-20% as compared to NLR.

![Figure 4.4: Comparison of RMSE of 4 hardening functions in predicting DP600 flow curves in the rolling direction](image)

Figure 4.4: Comparison of RMSE of 4 hardening functions in predicting DP600 flow curves in the rolling direction
The accuracy of each hardening equation is compared in terms of the adjusted R-squared value in Fig. 4.5a and RMSE in Fig. 4.5b. The adjusted R-squared values reveal that all the hardening functions considered can predict the strain and strain rate dependent flow behaviour of DP600 up to the uniform effective strain in an accurate way since the calculated $\bar{R}^2$ values are greater than 0.95. Among the hardening models investigated, the modified JC and the Voce-modified JC models are the most accurate while the power law and the Johnson-Cook models are the least accurate. In addition, KHL and the multiplicative combination of Voce–power law and Voce–Johnson Cook have approximately the same accuracy.

Figure 4.5: Cumulative (a) adjusted R-squared value and (b) RMSE calculated for DP600 in the RD testing direction

Figures 4.6 and 4.7 compare the predicted and experimental flow curves and hardening rates at strain rates 0.001, 1 and 100 s$^{-1}$ in terms of hardening evolution comparing with experimental uniaxial test results. One of the important observations is that almost all hardening equations underestimated the flow curve of DP600 at quasi-static strain rates, except the Voce–modified JC which accurately predicts the increases in the flow stress from one strain rate to another. In addition, Voce–type equations are more successful in predicting the yield stress while power law and the KHL functions underestimate it at low and high strain rates.

The evolution of the strain hardening rate ($d\sigma/d\varepsilon$) of this DP600 steel at different strain rates as well as the corresponding curves calculated by each hardening model are presented in Fig. 4.6b and 4.7b. This term is particularly important since it has a remarkable effect on the progress of local neck predicted by the Rousselier
micromechanical ductile damage model. All mentioned hardening laws predicted the overall slope of the stress–strain curves with an acceptable precision at different strains and strain rates. However, Voce–type models, can calculate the strain hardening rate in a better way at the beginning of deformation ($\varepsilon < 0.01$) compared with the other models. As a matter of fact, the latter hardening models exaggerate the hardening slope after the onset of yielding although it rapidly decreases to near actual values beyond a certain strain value.
Figure 4.6: Experimental and calculated true stress–strain curves and their corresponding slopes for DP600 sheet specimens at 0.001 s⁻¹
Figure 4.7: Experimental and calculated true stress–strain curves and their corresponding slopes for DP600 sheet specimens at 100s⁻¹
Apart from the different hardening models predicting different hardening rates at the beginning of the simulation, they also exhibit different strain hardening trends at high strain values. It can be seen in Fig. 4.8 that all hardening functions can reasonably predict the flow curve of DP600 at a strain rate of 0.1 s$^{-1}$ for the range of experimental data that is available (and this claim can be extended to the predictions at all strain rates). However, whilst Voce-like models approach null hardening rates and reach a saturation stress at large strains, other models almost reach a constant non-zero hardening rate after a certain amount of deformation. These different behaviours at large deformation are particularly important for predicting the onset of instability and the evolution of damage in a tensile specimen as they can strongly influence the necking geometry and final failure of the specimen. Furthermore, the large deformation behaviour will also have a significant effect on the outcome of numerical simulation of sheet metal forming processes.

Figure 4.8: Extended DP600 true stress–strain curves predicted by different hardening models at 0.1 s$^{-1}$
4.4.2 Finite element simulation

Calibration of Rousselier damage model

A necessary procedure for any ductile damage model is the calibration of material parameters and model coefficients. Four parameters need to be calibrated in the Rousselier model: $D$ and $\sigma_I$ as model constants, and $f_0$ and $\beta_c$. The initial void volume fraction can also be described by the fraction of eligible second phase particles (such as the martensite volume fraction in DP steels) that can be potential sites for void nucleation during the deformation, considering that not all of them take part in the nucleation process [29, 60, 61]. In addition, the void volume fraction at failure can be used instead of the critical scalar damage variable $\beta_c$ by using Eq. 4.1c. The initial void volume fraction was experimentally measured to be 0.07% by Winkler et al. [62] and $f_c = 0.1$ was determined by Abbasi et al. [63] and Ramazani et al. [12] and used in the current work.

Many simulations were carried out to determine $D$ and $\sigma_I$ at strain rates of 0.1 and 1 s$^{-1}$ and for each hardening equation, to determine whether or not changing these parameters has a significant effect on the performance of the Rousselier damage model for constant values of $f_0$ and $f_c$. Table 4.3 shows the sample ranges and arrangements of parameters and hardening models employed for these simulations. In each simulation, corresponding parameters in each associated row were used, and the reaction force and the displacement of the reference point was used to calculate the engineering stress–strain curve for further comparison. Python scripts were developed to automate the runs, derive related data points and post process the results. As it can be seen in Fig. 4.9, $D$ and $\sigma_I$ have negligible effects on the homogeneous deformation part of the flow curve, but they significantly affect the shape of the engineering stress–strain curve after maximum load is reached: i.e. higher values of parameter $D$ accelerate the progress of damage whereas increasing the value of $\sigma_I$ tends to postpone the failure by increasing the resistance to instability and failure.
Table 4.3: Design arrangement of parameters for the calibration process

<table>
<thead>
<tr>
<th>No.</th>
<th>$D$</th>
<th>$\sigma_I$ (MPa)</th>
<th>Strain–rate ($s^{-1}$)</th>
<th>Hardening model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.5</td>
<td>325</td>
<td>0.1</td>
<td>Power–law</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>325</td>
<td>0.1</td>
<td>Power–law</td>
</tr>
<tr>
<td>3</td>
<td>2.5</td>
<td>325</td>
<td>0.1</td>
<td>Power–law</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>325</td>
<td>0.1</td>
<td>Power–law</td>
</tr>
<tr>
<td>5</td>
<td>1.5</td>
<td>375</td>
<td>0.1</td>
<td>Power–law</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>32</td>
<td>3</td>
<td>475</td>
<td>1</td>
<td>Power–law</td>
</tr>
<tr>
<td>33</td>
<td>1.5</td>
<td>325</td>
<td>0.1</td>
<td>JC</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>48</td>
<td>3</td>
<td>475</td>
<td>0.1</td>
<td>JC</td>
</tr>
<tr>
<td>49</td>
<td>1.5</td>
<td>325</td>
<td>1</td>
<td>JC</td>
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<td>...</td>
</tr>
<tr>
<td>65</td>
<td>1.5</td>
<td>325</td>
<td>0.1</td>
<td>modified–JC</td>
</tr>
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<td>...</td>
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<td>...</td>
</tr>
<tr>
<td>97</td>
<td>1.5</td>
<td>325</td>
<td>0.1</td>
<td>Voce–mJC</td>
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<td>...</td>
</tr>
<tr>
<td>160</td>
<td>3</td>
<td>475</td>
<td>1</td>
<td>KHL</td>
</tr>
</tbody>
</table>

Figure 4.9: Comparison of experimental and predicted DP600 flow curves at 0.1 s$^{-1}$ with different $D$ and $\sigma_I$ using the (a) KHL and (b) modified–JC hardening models

Based on simulation results, $D = 2$ and $\sigma_I = 450 \pm 5$ MPa for Voce–type functions, and $D = 2.5$ and $\sigma_I = 390 \pm 15$ MPa for power law–type models are obtained in order to achieve the optimized Rousselier model parameters and the best fit of the engineering
stress–strain curve comparing to experiments. To avoid complication and compare the simulation results with experiments at constant damage parameters, the average values predicted for $D$ and $\sigma_I$ among all cases were used for the simulations, as presented in Table 4.4. The result of the calibrating procedure for KHL ($\sigma_I = 400$ MPa), modified–JC ($\sigma_I = 385$ MPa) and Voce–modified JC ($\sigma_I = 450$ MPa) are shown in Fig. 4.10.

![Figure 4.10: Comparison of experimental and predicted engineering stress–strain curve for DP600 at 0.1 s$^{-1}$ calculated based on different hardening models](image)

Table 4.4: Rousselier damage model parameters of DP600

<table>
<thead>
<tr>
<th>$D$</th>
<th>$\sigma_I$ (MPa)</th>
<th>$f_0$ [62]</th>
<th>$f_c$ [63]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>425</td>
<td>0.0007</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Simulation results

In the Rousselier damage model, the evolution of $\beta$ and $f$ need to be carefully assessed. Figures 4.11 and 4.12 show the evolution of $\beta$ and $f$ from the beginning of the deformation up to failure in the centre of the tensile specimens at low (0.1 s$^{-1}$) and intermediate (100 s$^{-1}$) strain rates, respectively. The results indicate that under
quasi-static conditions (Fig. 4.11a and 4.12a), there are no obvious differences in the evolution of $\beta$ and $f$ when predicted by different hardening models up to a certain strain level at the centre of the specimens. The void volume fraction is negligible up to 0.6 strain, then it begins to increase gradually between 0.6 and 0.8 strain, and subsequently, increases to $f_c = 0.1$ through to the end of the tensile test. However, these trends at large strains ($\varepsilon_p \geq 1.0$) are dependent on the hardening model in quasi–static conditions, where the final strain value predicted by Voce–type models is slightly greater than that predicted by other models. The same behaviour can also be observed for other strain rates (Fig. 4.11b and 4.12b), i.e. all hardening equations result in the same pattern of damage growth, although the mentioned small deviations in the damage growth behaviour starts at lower strains. It is worth noting that the growth in the scalar damage parameter is the same for $\dot{\varepsilon} = 0.1 \text{ s}^{-1}$ and $\dot{\varepsilon} = 100 \text{ s}^{-1}$ (Fig. 4.11a,b) up to $\varepsilon \simeq 0.4$ and after that the trend changes slightly through the rest of deformation. The reason is that the flow curve obtained from an ASTM (E8M-04) and miniature dog–bone specimens are comparable until the maximum load but after that, i.e. in the non–uniform plastic deformation area, they are not identical, as explained by Bardelcik et al. [64] and Rahmaan et al. [8].
Figure 4.11: Variation of scalar damage variable ($\beta$) vs. equivalent plastic strain, calculated by Rousselier damage model and different hardening equations at low and high strain rates

(a) $\dot{\varepsilon} = 0.1s^{-1}$

(b) $\dot{\varepsilon} = 100s^{-1}$
Figure 4.12: Variation of void volume fraction ($f$) vs. equivalent plastic strain, based on different hardening equations at low and high strain rates.

Another approach to investigate the void volume fraction during the deformation is to evaluate its behaviour throughout the time of the process. Fig. 4.13 presents the
history of void volume fraction throughout the normalized time of the simulation, i.e. normalized to the total time of the deformation up to complete failure. Void volume fraction is approximately zero at the beginning of simulation and it remains the same until a certain time when it rises sharply to final void volume fraction at failure. As it can be seen in Fig. 4.13a and 4.13b the general trend in which $f$ increases from 0 to $f_c$ is the same for all strain rates and for all hardening equations. Therefore, the rate of void growth, in this model, is independent of the constitutive equation and of the strain rate. Having said this, the time at which the void growth commences, is very different depending on the strain rate and the hardening rule utilized in the model. This behaviour can be correlated with the hardening rate at high strain values, as shown in Fig. 4.8. The hardening rate is representative of the resistance of the material against softening which consequently has an influence on its load bearing capacity. Thus, hardening models that exhibit higher strain hardening rates at large strains tend to decelerate and postpone the material softening that is caused by damage growth. Therefore, the order in which the hardening rate alters from Voce-like models (lowest) to JC (highest) in Fig. 4.8 is exactly the same order in which the onset of sudden void growth occurs, as indicated in Fig. 4.13a. Likewise, the same explanation can be extended to the behaviour of void growth at high strain rate (Fig. 4.13b). In addition, it can also be observed from Fig. 4.13c that the starting time of void volume fraction growth is reduced by increasing the strain rate for a given hardening function.
Figure 4.13: History of the evolution of void volume fraction based on different hardening functions (a) at $\dot{\varepsilon} = 0.1 \text{s}^{-1}$ and (b) at $\dot{\varepsilon} = 100 \text{s}^{-1}$ (c) comparison of void evolution history at different strain rates using modified–JC and Voce–modified JC hardening laws

The strain distribution in the tensile specimen and the geometry of the neck after the moment when maximum load was reached and diffuse necking was initiated, were predicted at different strain rates using different hardening models and were qualitatively compared with experimental results obtained using DIC. The results of this study are shown in Fig. 4.14. It can be seen that all quasi-static specimens experienced diffuse necking and all specimens displayed strain localization at the centre of the gauge area. But there are differences in the strain distribution around the neck, as predicted by the different hardening models implemented in the Rousselier damage model. At 0.1 $\text{s}^{-1}$, shown in Fig. 4.14a, the modified Johnson-Cook and JC models
show the most uniform deformation gradient across the local neck at the same level of equivalent plastic strain at the centre of the neck ($\varepsilon_{eq}^p \approx 0.6$). The most severe shear bands can be seen in the middle of specimens whose strain distribution was predicted with a Voce–type function, and where the stress is confined to a saturated value. This causes the strain to be more localized in shear bands and for localization to start sooner, as can also be seen in Fig. 4.13. At strain rates of 1 and 100 s$^{-1}$, the onset of instability occurred in the middle of the specimen but the intensity of localization in shear bands is reduced compared with the quasi-static condition. Considering the strain distribution contours in Fig. 4.14, it can be understood that the intensity of strain localization at each level of strain rate also follows the strain hardening rate predicted by each hardening equation. This means that the JC model with the greatest hardening rate among investigated models shows the least localized deformation around the neck whereas the multiplicative Voce models predict more severe localization at the centre of the specimens. Comparing the deformation outside the neck in the uniformly deformed area, also confirms this hypothesis. Since the material defined by Voce-like models cannot show any resistance to the flow softening caused by void evolution in micromechanical damage models (due to stress saturation), the predicted uniform elongation decreases compared with other models that can withstand the softening process and help to maintain a more homogeneous deformation throughout the specimen.
Figure 4.14: Strain distribution along uniaxial tensile test specimens at the onset of necking, using different hardening models comparing to experimental results at (a) 0.1, (b) 1.0 and (c) 100 s⁻¹

The geometry of the damage in the tensile specimens deformed at 0.1 and 100 s⁻¹ is presented in Fig. 4.15. Localization and failure start at the centre of all specimens and,
subsequently, elements are removed from the simulations. However, the propagation of failure differs depending on the hardening equation and the strain rate. Based on Fig. 4.15(a), although all models show localization on the shear bands in the quasi-static specimens, the damage front progresses directly toward the edge of the specimen in case of modified-JC and KHL but it advances along the shear bands when using Voce–power law and Voce–modified JC in the simulation, as shown by the arrows in the figure. Therefore, at low strain rate, the final geometry of the damaged area is predicted to be a normal diffuse neck that would lead to ductile fracture using the former models, whereas the latter functions exhibit more localized necking and damage on the shear bands, which can again be explained in terms of the strain hardening trend determined by each hardening model. If the full geometry model was used instead of the quarter-symmetry, as described in Section 4.3.4, the damage would take place in an X-shape and fracture could occur on either of the shear bands using Voce-type hardening functions.

At moderate and high strain rates, all models predicted the failure to propagate from the centre to the edge of the specimen, perpendicular to the loading direction, as shown by arrows in Fig. 4.15(b). This can be attributed to the geometry of the miniature specimen and the flow behaviour predicted by the hardening function utilized in the Rousselier model. The fracture configuration, relative to specimen symmetry axes, predicted by Voce-type models at low strain rate and all models at strain rate 100 s\(^{-1}\) are in good agreement with experiments, as can be observed in Fig. 4.15.
4.5 Conclusions

This research presents a complete study of uniaxial tensile flow behaviour of DP600 at different strain rates from quasi-static to high strain rate. A new optimized technique based on a combination of non-linear regression and the Markov chain Monte Carlo method (MCMC) is proposed to fit different hardening equations to experimental data.
points. A user material subroutine was developed to employ Rousselier continuous ductile damage model and hardening functions to simulate the tensile tests using ABAQUS/Explicit finite element software. Based on numerical simulation results and comparing them with experiments, the following conclusions can be drawn:

1. The proposed NLR+MCMC fitting procedure can accurately determine all the fitting parameters in the hardening equations. This approach is computationally efficient and fast comparing to other optimizing methods.

2. All investigated strain–strain rate hardening models could successfully predict the flow behaviour of DP600. Among all, the modified Johnson-Cook and multiplicative combination of Voce–mJC exhibited the greatest accuracy. However, each hardening function showed different strain hardening rate behaviour when extrapolated to large strains.

3. The Rousselier model is a ductile damage model that can precisely predict the material response in uniaxial tension. It is shown that the increase in the scalar damage variable and consequent void growth, predicted by the Rousselier model, is reasonably independent of the hardening law at low and moderate strains at different strain rates up to a certain strain value, however, the onset of rapid void growth depends somewhat on the hardening function and the way it predicts the hardening rate at large strains. Higher hardening rates, as seen in the power law, JC and KHL models, result in postponing the time of sudden void volume increase while Voce–type models cause this sudden damage to occur earlier.

4. All hardening equations implemented in the Rousselier damage model demonstrate good capabilities in predicting the strain distribution along the gauge length of the specimens at different strain rates. Despite some variations, simulation results were consistent with the experimental strain map obtained using DIC technique. Voce models in quasi-static, and modified JC in low and high strain rates could exhibit better results in terms of the average plastic strain in the neck and in uniformly deformed areas of the gauge.

5. Although all hardening models predicted the onset of strain localization from the centre of the gauge section, the progressive development of damage can be
very different. In the quasi-static conditions, strain localized on the shear bands and the consequent fracture is better predicted by the combination of Rousselier model and Voce-like hardening functions. However, radial damage as well as ductile fracture are predicted by other hardening functions.

6. Based on numerical simulations, it has been shown that the strain hardening rate at large strain values, at a given strain rate, plays an important role in predicting the deformation behaviour of a sheet material. Therefore, uniaxial tensile test data is not sufficient to validate a numerical model; therefore, performing other mechanical tests, such as hydrostatic bulge tests, to obtain the deformation behaviour of a material under different forming modes appears to be necessary.

Acknowledgments

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4.6 Bibliography


Chapter 5

Damage evolution and void coalescence in finite-element modelling of DP600 using a modified Rousselier model

In this chapter, numerical simulations of uniaxial tensile deformation of DP600 steel were carried out using a modified Rousselier ductile damage model at different strain rates ranging from 0.1 to 100 s\(^{-1}\). Since the original Rousselier model does not consider any secondary void nucleation or coalescence criteria, it was modified by including a strain-controlled void nucleation function, a coalescence criterion and a void growth acceleration function as the post-coalescence regime identifier. The predicted flow behaviour, the evolution of damage and critical strain and void volume fraction at the onset of coalescence were assessed to evaluate the performance of the proposed model at each strain rate. In addition, X-Ray tomography analysis was employed to evaluate the void volume fraction predicted by each void coalescence criterion. The modified Rousselier model showed good agreement with the experimentally determined strain and void volume fraction at the onset of coalescence. Also, it could successfully predict the damage distribution and the final damage geometry of DP600 tensile specimens.
5.1 Introduction

Prediction of damage and failure in engineering materials and structures is a challenging field of research that has gained a lot of attention in both academia and industry. Accurate assessment of structural integrity of sheet metal products by numerical analysis, with regard to the development of new high performance materials, is of great importance since it can contribute to higher design efficiency, and more cost and time effectiveness [1]. Sheet metals can exhibit different forming and failure behaviour depending on the loading conditions such as the strain path and strain rate. Therefore, it is essential to utilize an accurate hardening law, ductile damage model and fracture criterion in numerical simulations to accurately reproduce experimental behaviour.

The use of dual phase (DP) steels is rapidly growing in the automotive industry due to their superior performance in terms of combined ductility, work hardening rate, strength-to-weight ratio and crash resistance. Their microstructure usually consists of 5-30 vol% martensite, responsible for strengthening the material, distributed in a ductile ferrite matrix which accommodates the deformation throughout the forming process [2–4]. Tasan et al. [5] investigated the effect of microstructural properties of a dual phase steel on the localization and damage mechanisms for different strain paths. Besides conventional low strain rate forming processes used to deform these steels, such as stamping and hydroforming, there is an increasing interest in the automotive industry to utilize high strain rate deformation processes, such as electromagnetic or electrohydraulic forming, which can result in significantly higher formability [6, 7]. Experimental research has shown remarkable improvement in the formability of DP500, DP600, DP780 and DP980 steel sheets that were subjected to electrohydraulic deformation process [7, 8]. In addition, Amirmaleki et al. [9] used the representative volume element (RVE) method to model the flow behaviour of DP500 and bainite-aided DP600 steels. Accordingly, developing a complete micromechanical damage model based on precise constitutive equations, void nucleation and void growth functions, and a void coalescence criterion would help to predict the hardening, instability and damage behaviour of investigated DP steel in a wide range of strain rates, from quasi-static conditions to high strain rates.
A micromechanical approach to ductile failure relates the damage of most engineering alloys to nucleation of microvoids during the deformation because of crack initiation at second phase particles or at the interface between hard particles and the ductile matrix. As the deformation progresses, voids grow as a result of increasing strain and consequently, the load bearing capacity of the material progressively decreases until coalescence of cavities leads to complete failure [10, 11]. McClintock [12], and Rice and Tracey [13] were among the first researchers to describe the growth of a cylindrical or spherical void in an infinite deforming ductile material with no strain hardening. In these early models, no interaction between voids and the coalescence process was considered, and failure was simply linked to the critical value of the void radius. Later, various thermodynamically consistent models, based on porous material plasticity, were proposed and the best known are those developed by Gurson [14], Gurson-Tvergaard-Needleman (GTN) [15, 16], Rousselier [17, 18] and Lemaitre [19]. GTN is perhaps the most widely-used model to evaluate the forming and failure behaviour of different materials in different forming processes, and it can predict void initiation, growth and coalescence using a void growth acceleration function. Chen and Dong [20] employed a modified GTN model accompanied by Hill’s quadratic yield criterion to evaluate the damage in plane strain tension and deep drawing. Butcher et al. [21] used this model to predict the onset of fracture in tube hydroforming of DP600. Ramazani et al. [2] derived the flow limit curve of a DP steel deformed in a cross-shaped die. However, the original Gurson model and the version modified by Tvergaard and Needleman are not able to predict the damage for zero or negative stress triaxiality ($\sigma_m/\sigma_{eq}$) values, e.g. in pure shear deformation. Some researchers have proposed improved versions of GTN damage model in order to overcome this deficiency [22–24], although Bao and Wierzbicki acknowledged that it is difficult to define a damage model that is capable of predicting the damage behaviour of a material for different stress triaxialities [25].

The Rousselier model has also been used in several studies to model the deformation and damage behaviour of materials in terms of void evolution. Besson et al. [26] used the Rousselier function to model crack growth and formation of cup-cone fracture surfaces; Poussard et al. [27] employed it to simulate the damage in smooth tensile and compact
tension specimens. Samal and Shad [28] predicted the fracture resistance behaviour of cracked fuel pin specimens using this model; and Tu et al. [29] simulated the fracture and crack propagation in steel electron-beam-welded joints and aluminium laser-welded joints. Despite some similarities between the GTN model and the Rousselier model, there are some important differences between them. In case of very low, zero or negative stress triaxiality, the Rousselier model allows damage to initialize and grow whereas in GTN, no damage growth can be generated. In addition, the GTN model was developed based on the growth of a spherical or cylindrical shaped void in the material, whereas Rousselier did not establish his model based on any particular void shape. Therefore, it is possible for the Rousselier model to capture the transition from a flat to oblique fracture surface without any additional term or further modifications [30, 31]. However, the original Rousselier model does not include any void nucleation function, or coalescence criterion that would trigger coalescence based on a critical void volume fraction [30]. Recently, Zanganeh et al. [32] proposed an approach to couple the Rousselier model and a coalescence criterion and evaluated the model for different positive triaxiality levels using notched specimens in uniaxial tension of AA2050. Moreover, Rousselier et al. [33] employed the Rousselier damage model along with a strain controlled void nucleation function to evaluate the damage accumulation in Al6260 thin-walled extrusion alloy and Al2XXX alloy. In view of the advantages of the Rousselier damage model, it was used to evaluate the tensile behaviour of a DP600 steel sheet.

In this research, finite element analysis was used to analyse the uniaxial tensile flow, instability and damage behaviour of DP600 at quasi-static, intermediate and high strain rates. In order to define the hardening behaviour of DP600, three different rate sensitive hardening constitutive equations were fitted to experimental uniaxial tensile data. Subsequently, an appropriate void nucleation function, a void coalescence criterion and a void growth acceleration function were combined with the Rousselier damage model. The implementation of various criteria to build a complete Rousselier model is similar to the work of Zhang et al. [36] who coined the expression “The Complete Gurson Model Approach”. The comprehensive model was then implemented in a user material subroutine (VUMAT) to be used in ABAQUS/Explicit finite element
simulation software. The effects of the hardening function, void nucleation function and void coalescence criterion on the prediction of the flow and damage behaviour of DP600 at different strain rates, are assessed and discussed.

5.2 Material model

5.2.1 Rousselier damage model

The Rousselier model \cite{17, 18} is an elasto-plastic, continuous ductile damage model that assumes isotropic-hardening and isotropic-damage during the deformation of a material and is based upon the decomposition of the free Helmholtz potential energy ($\Phi$) into stored elastic energy ($\Phi_e$), stored plastic energy ($\Phi_p$) and stored damage energy ($\Phi_d$) \cite{30, 37},

$$\Phi(\varepsilon_e, \varepsilon_p, f) = \Phi_e(\varepsilon_e) + \Phi_p(\varepsilon_p) + \Phi_d(f) \quad (5.1a)$$

where $\varepsilon_e$, $\varepsilon_p$ and $f$ are the elastic strain, plastic strain and the porosity volume fraction, respectively. The plastic potential, proposed by Rousselier \cite{18}, is an extension of the von Mises yield criterion with an additional term which describes the damage as the growth of voids in a ductile material:

$$\Phi = \frac{\sigma_{eq}}{1 - f} - R + B(\beta)D \exp\left(\frac{\sigma_m}{(1 - f)\sigma_1}\right) = 0 \quad (5.1b)$$

where $\sigma_{eq}$ is the von Mises equivalent stress, $\sigma_m$ is the hydrostatic stress and $R$ is the true stress-strain curve of the material. $f_0$ and $f$ are the initial and current void volume fraction, respectively. $B(\beta)$ is the conjugate force to the scalar damage parameter ($\beta$), and $D$ and $\sigma_1$ denote adjustable material parameters which are responsible for damage acceleration or resistance to growth and coalescence of voids. The damage variable $\beta$ is directly related to the plastic multiplier in the normality rule ($\lambda$) or the
plastic strain increment ($\dot{\varepsilon}_p$) and helps material softening surpass the hardening in the final steps of deformation until the material completely loses its load-bearing capacity:

$$\dot{\beta} = \dot{\varepsilon}_p D \exp \left( \frac{\sigma_m}{(1 - f)\sigma_1} \right)$$

(5.1c)

The relation between the damage parameter $\beta$, $f$ and $f_0$ is given by:

$$\beta = \ln \left( \frac{f}{1 - f} \times \frac{1 - f_0}{f_0} \right)$$

(5.1d)

It is worth noting that in the original Rousselier model, neither secondary void nucleation nor any particular critical void volume fraction at coalescence or failure was assumed $^{30}$ $^{32}$. Therefore, void nucleation was defined by the fraction of second phase particles present in the material and void growth ($df_g$) was considered as the main mechanism for void evolution ($df$), as shown in Eq. 5.1e

$$df = df_g, \ f(0) = f_0$$

(5.1e)

5.2.2 Hardening models

Defining the hardening behaviour of materials by either phenomenological or physically based constitutive equations is particularly important in the simulation of forming processes and damage evolution since each hardening model predicts the hardening rate ($d\sigma/d\varepsilon$), at large strains, in an entirely different manner based on its origins, although most of them can accurately predict the stress-strain curves at low strain ranges $^{38}$ $^{41}$. In addition to the strain hardening behaviour, it is essential for a function to be able to account for the strain rate sensitivity of materials in order to accurately predict their dynamic behaviour. Based on strain hardening behaviour, hardening functions can either reach a saturation stress or zero strain hardening rate, or exhibit unbounded hardening rate at large strains $^{42}$. 
Among many hardening functions proposed in the literature for different materials, applications and forming processes, the following three equations were implemented in the Rousselier damage model:

1. **modified Johnson-Cook**: The Johnson-Cook model \[43\] is one of the well-known elastoplastic hardening functions, used to determine the flow behaviour of various materials including DP steels such as DP590 \[44\], DP780 \[45\], and DP1200 and DP1400 \[46\], as a function of strain-rate and temperature. There are many versions of the JC function in the literature, in which the temperature part of the function has been modified \[46, 47\]. Since it is shown that the strain rate sensitivity of a material cannot accurately be captured by a linear function of natural log \[48\], another constant \((C_5)\) is now added to the strain-rate sensitive part of original form of the JC model to improve its ability to predict the dynamic behaviour of DP600 steel sheets (Eq. 5.2a).

2. **Voce-modified Johnson-Cook**: The Voce equation \[49\] is the most important “saturation” hardening model, used to describe the work hardening behaviour of materials. Cao et al. \[50\] used it to define the tensile flow curve of DP800. Since the original form of the Voce function is not rate dependent, a new multiplicative combination of the Voce strain hardening function, and the modified Johnson-Cook strain-rate sensitive function, shown in Eq. 5.2b, was employed in this study.

3. **Khan-Huang-Liang (KHL)**: KHL \[51, 52\] is one of the most important constitutive hardening models, used to define the flow behaviour of different engineering materials over a wide range of strain rates \[53, 54\]. In this model, the strain hardening is associated with strain rate. Moreover, the hardening rate is unbounded at large strains but it does not change with temperature \[42\]. The KHL equation is shown in Eq. 5.2c.
\[ R = (C_1 + C_2 \varepsilon_p) \left[ 1 + C_4 \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \right] \]  
(5.2a)

\[ R = C_1 - (C_1 - C_2) \left( 1 - \exp(-C_3 \varepsilon_p) \right) \left[ 1 + C_4 \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \right] \]  
(5.2b)

\[ R = \left[ C_1 + C_2 \left( 1 - \frac{\ln \dot{\varepsilon}_p}{\ln D_0^p} \right)^{C_4} \left( \frac{\varepsilon_p}{\varepsilon_0} \right)^{C_3} \right] \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right)^{C_5} \]  
(5.2c)

In Eq. 5.2, \( C_{1...n} \) are material constants, \( \dot{\varepsilon}_0 \) is the reference strain rate and is equal to 1 s\(^{-1}\), and \( D_0^p \) denotes an arbitrary upper bound strain-rate (usually chosen as \( 10^6 \) s\(^{-1}\)). It is worth noting that the temperature-dependent term of the original functions was omitted since conventional forming processes as well as all experimental tests in this study were carried out at ambient temperature.

### 5.2.3 Void nucleation

The original form of the Rousselier damage model does not include any void nucleation function but it assumes cluster nucleation (CN) where the initial void volume fraction remains constant (\( f_0 = \text{cte.} \)). Although cluster nucleation and continuous nucleation (\( df_N = A_0 \, d\varepsilon_p \)) models have been used to simulate the damage behaviour of aluminium\(^{32,55}\) and steel\(^{56}\), it is shown that employing a void nucleation function that is controlled either by strain, stress or hydrostatic stress, can make a model more precise and more realistic (\( df = df_g + df_N \))\(^{15}\). Generally, stress-controlled void nucleation is used for materials with large particles that tend to crack, and strain-controlled void nucleation (SCVN) is more suited to materials with small particles that tend to debond\(^{21,57,58}\). Although both strain and stress-controlled nucleation models can be used for DP600 due to the size of its martensite particles, both Butcher et al.\(^{21}\) and Ramazani et al.\(^2\) showed that strain-controlled void nucleation could lead to more accurate results compared to experiments. The controlled void nucleation function, used in this study can be written as:
\[ df_n = A \, d\varepsilon_p + B \, d\sigma_{eq} + C \, d\sigma_m \]  
\[ A = \frac{f_N}{S_N\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{S_N} \right)^2 \right] \]  
\[ B = C = 0 \]

where \( df_n \) is the first derivative of the porosity distribution with respect to time; \( f_N \), \( \varepsilon_N \) and \( S_N \) are the volume fraction of void nucleating particles, the mean value of the normal distribution of nucleating strain and the standard deviation, respectively.

### 5.2.4 Void coalescence criteria

Coalescence can be defined as the rapid linking of voids to build a microcrack in the material which contributes to a sudden decrease in the load-bearing capacity and final failure. In the Gurson model, a critical void volume fraction \((f_c)\), considered to be a material constant, determines the onset of coalescence and sudden material capacity loss \([16]\). However, it has been pointed out that \( f_c \) strongly depends on the initial void volume fraction \((f_0)\) and on the strain path \([36]\). Accordingly, the plastic limit-load model (PLL) proposed by Thomason \([57, 59]\) has become a more acceptable criterion for identifying the onset of coalescence. The concept of this model lies in two competitive modes of deformation: stable homogeneous and unstable localized. In the early stages of deformation, void volume fraction is low and it is easier to achieve homogeneous deformation. Nevertheless, the stress required for localized deformation decreases by void nucleation and growth during the deformation. Based on this criterion, when the stress required for homogeneous deformation and that of localized deformation become equal, coalescence occurs, the plastic limit-load is reached, the deformation will localize between neighbouring voids, and the current void volume fraction can be considered as the critical void volume fraction at the onset of coalescence \((f_c)\). Many researchers extended Thomason’s model to include the effect of material properties, cell geometry \([60, 61]\) and void shape \([62]\). Zhang et al. \([36]\) wrote the Thomason plastic limit-load criterion for a 3D deformation system as follows:
\[ \frac{\sigma_I}{\sigma_{eq}} = \left[ \alpha_t \left( \frac{1}{\chi} - 1 \right)^2 + \frac{\beta_t}{\sqrt{\chi}} \right] \left( 1 - \pi \chi^2 \right) \] (5.4a)

\[ \chi = \left( \frac{3f}{4\pi} \exp(\varepsilon_I + \varepsilon_{II} + \varepsilon_{III}) \right)^{1/3} \left( \frac{(\exp(\varepsilon_{II} + \varepsilon_{III}))^{1/2}}{2} \right)^{-1} \] (5.4b)

where \( \sigma_I \) is the maximum principal stress, \( \alpha \) and \( \beta \) are model constants, \( \chi \) represents the void space ratio, and \( \varepsilon_{I,II,III} \) denote principal strains. Another representation of Thomason’s model can be found in Pardoen et al. [61] and Scheyvaerts et al. [63]:

\[ \frac{\sigma_I}{\sigma_{eq}} = \left[ \alpha_t \left( \frac{1}{W \chi} - 1 \right)^2 + \frac{\beta_t}{\sqrt{\chi}} \right] \left( 1 - \eta \chi^2 \right) \] (5.5)

where \( W \) and \( \eta \) are the void aspect ratio (\( W=1 \) for spherical voids) and a geometric factor based on void arrangement and void cell geometry (\( \eta=1 \) for cylindrical cell geometry), respectively. Although \( \alpha_t \) and \( \beta_t \) were defined as constants in Thomason’s original model, Pardoen and Hutchinson [60] redefined the former parameter as a function of strain hardening exponent \( n \) in the power law hardening function in order to take the hardening behaviour of the material into account. Their calculations based on large numbers of axisymmetric finite element cell calculations indicated that \( \alpha_t = 0.1 + 0.217n + 4.83n^2 \) for materials with \( 0 \leq n \leq 0.3 \) and \( \beta_t \simeq 1.24 \). Benzerga et al. [62] also improved the performance of the Thomason’s coalescence model using four axisymmetric velocity fields from the Lee–Mear expansion and extended it for wider range of void shapes:

\[ \frac{\sigma_I}{\sigma_{eq}} = 0.1 \left( \frac{\chi^{-1} - 1}{W^2 + 0.1\chi^{-1} + 0.02\chi^{-2}} \right)^2 + \frac{1.3}{\sqrt{\chi}} \] (5.6)

Another approach to calculate the void space ratio, i.e. the ligament size ratio (\( \chi \)) was proposed by Chambert et al. [64] based on a cylindrical unit cell with a height \( 2H \) units and a base of radius \( R \) units, which contains a spherical void with radius \( r \). Initial values for the height and radius of the cell are \( H_0 \) and \( R_0 \), respectively. Combined with a unit cell aspect ratio (\( \gamma = 2/3 \) for an axisymmetric unit cell) defined by Chen and Butcher [58], the relation between \( \chi \) and geometrical parameters can be
written as:

\[ \chi = \frac{r}{R} = \left( \frac{f}{\gamma} \vartheta \right)^{1/3} \]  \hspace{1cm} (5.7a)

\[ \vartheta = \frac{H}{R} = \vartheta_0 \exp \left( \frac{1}{\gamma} \varepsilon_{eq}^p \right) \]  \hspace{1cm} (5.7b)

\[ \vartheta_0 = \frac{H_0}{R_0} \]  \hspace{1cm} (5.7c)

where \( \vartheta \) and \( \vartheta_0 \) are the current and initial void distribution parameter, respectively.

### 5.2.5 Post coalescence regime

When the void volume fraction in the material reaches a critical value \( (f_c) \), coalescence begins and the load-bearing capacity of the material starts to decrease rapidly. As the void volume fraction continues to increase, it reaches the critical value \( (f_F) \) when final fracture or complete failure occurs \[16\]. Having derived the critical void volume fraction at coalescence using the coalescence criterion, the effective void volume fraction \( (f^*) \) can be defined by a void growth acceleration function, which is given by:

\[ f^* = \begin{cases} f & \text{if } f \leq f_c \\ f_c + \delta (f - f_c) & \text{if } f \geq f_c \end{cases} \]  \hspace{1cm} (5.8a)

\[ \delta = \frac{f_u^* - f_c}{f_F - f_c} \]  \hspace{1cm} (5.8b)

where \( \delta \) and \( f_u^* \) are the phenomenological multiplicative void growth acceleration factor and final effective void volume fraction when \( f = f_F \), where the load bearing capacity decreases to zero, respectively \[20\] \[21\].

### 5.2.6 Implementation procedure

After the onset of plastic deformation and at each time increment, the Rousselier integration procedure, described explicitly by Shterenlikht \[65\], is used to determine
the correct value of the equivalent plastic and hydrostatic strain increments ($\Delta \varepsilon_{eq}^p$ and $\Delta \varepsilon_{m}^p$) as well as the strain ($\varepsilon_{ij}$) and stress ($\sigma_{ij}$) tensors. Subsequently, $\sigma_{eq}$, the maximum principal stress ($\sigma_I$), the current value of scalar damage variable ($\beta$) and the void volume fraction ($f$) are calculated with regard to the void nucleation function. In the next step, the local strength, which is the right hand side (RHS) of Eq. 5.4a or 5.5, and the homogeneous strength ($\sigma_I/\sigma_{eq}$) are compared with each other and three possible cases are considered:

- **$RHS > \sigma_I/\sigma_{eq}$**: since the stress required for local deformation mode is greater than that of homogeneous mode of deformation, no coalescence or void growth acceleration occurs.

- **$RHS = \sigma_I/\sigma_{eq}$**: coalescence criterion is satisfied under this condition so the current void volume fraction is considered as the critical value at the onset of coalescence ($f_c$).

- **$RHS < \sigma_I/\sigma_{eq}$**: coalescence has already started, and therefore the void volume fraction should be calculated based on the void growth acceleration function (Eq. 5.8) and the Rousselier damage variable ($\beta$) needs to be redetermined based on the post-coalescence effective porosity value ($f^*$) via Eq. 5.1d.

Complete loss of load carrying capacity and total failure takes place when the void volume fraction reaches its critical value at rupture ($f = f_F$) or the effective post-coalescence porosity value reaches its ultimate value ($f^* = f_{u}^*$). Figure 5.1 shows a flowchart of this procedure for implementing the void nucleation and coalescence models into the ABAQUS user material subroutine.

## 5.3 Methodology

### 5.3.1 Material

The material studied was a DP600 sheet with a nominal thickness of 1.49 mm and 92.0, 4.7 and 3.3 vol% of ferrite, martensite and bainite, respectively. Table 5.1 presents
Figure 5.1: Flowchart of the implementation of void nucleation and coalescence in the model
Table 5.1: Chemical analysis of as-received DP600 steel (% in weight)

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>Cr</th>
<th>Mo</th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.107</td>
<td>1.5</td>
<td>0.18</td>
<td>0.18</td>
<td>0.21</td>
<td>0.06</td>
<td>0.04</td>
</tr>
</tbody>
</table>

the chemical composition of the investigated DP600 sheet.

5.3.2 Experimental procedures

Uniaxial tensile tests were carried out on DP600 sheets using 2 different specimen geometries: an ASTM (E8M-04) specimen for quasi-static conditions (0.001 and 0.1 s\(^{-1}\)) and a miniature “dog-bone” specimen for intermediate strain rate experiments (1, 10, 100 s\(^{-1}\)). An Instron model 1331 servo-hydraulic testing machine and a Hydraulic Intermediate Strain Rate (HISR) apparatus, developed at the University of Waterloo \[67\], were employed to perform uniaxial tensile tests at strain rates of 1 s\(^{-1}\) and below, and higher than 1 s\(^{-1}\), respectively. To obtain strain rates from 0.001 to 100 s\(^{-1}\), tests were performed with cross-head velocities of 3, 300, 750, 19500 and 180000 mm/min. For quasi-static strain rates, a \(\pm 12.5\) biaxial extensometer was used to measure the axial and width strains of the specimens, while Digital Image Correlation (DIC) technique accompanying a virtual extensometer were employed to measure experimental strain distribution along the gauge area of the sub-size tensile specimens. Data processing of obtained images from the high speed video image acquisition was performed using Vic-2D software from Correlated Solutions Inc in order to measure the longitudinal and width strain of the miniature-tensile specimens.

After calculating the engineering stress by dividing the measured force by the original cross-sectional area of the gauge, and the true (plastic) strain from the DIC results, the true stress-true plastic strain curve as well as the engineering flow curve were constructed for each strain rate \[68\]. The true flow curves were used to obtain hardening function fitting parameters. A detailed description of the testing procedures, specimens, tools, measurement techniques and the results for these experiments has been published by Thompson \[69\] and Rahmaan et al. \[68\].
5.3.3 Finite element model

To model the uniaxial tensile test, only a quarter of the geometry of the ASTM (E8M-04) and miniature dog-bone specimens, shown in Fig. 5.2 were modelled due to the symmetrical nature of the deformation. The Rousselier ductile damage model was modified to include a strain controlled void nucleation function, void coalescence criteria and the hardening equations. The model was implemented into the ABAQUS/Explicit finite element simulation software as a user material subroutine (VUMAT), following the integration procedure developed by Shterenlikht [65].

The size of the grip section of both specimens was reduced to decrease the computational cost and simulation time. A reference point was considered a few millimetres above the grip section such that all degrees of freedom were constrained, except in the velocity direction. The top surface of the grip section was coupled to the reference point in the direction of motion, and the experimental velocities for each strain rate, were applied to this reference point. Nodal displacement along the symmetry line perpendicular to the specimen axis, in the centre of gauge area, were locked in the loading direction and symmetric boundary conditions were applied along the symmetry axes of the specimen, i.e. parallel to the loading direction. The reaction force and the displacement of the reference point were derived to calculate the engineering flow curves of the specimens in each condition.

It has been stated by several researchers that the mesh size has a significant influence on the slope of the flow curve after the onset of localization [31, 70]. Therefore, mesh dependency assessment was performed by reducing the mesh size from 0.5 mm to 0.1 mm for quasi-static specimens and from 0.3 mm to 0.05 mm for the miniature dog-bone geometry. Reduced integration 8-node brick elements (C3D8R) were used to mesh the specimens at different strain rates. Since the gauge area of the miniature intermediate and high strain rate specimen are considerably smaller in size, it is necessary to reduce the element size for these specimens in order to maintain a uniform element aspect ratio. Simulation results showed that a reasonably fine element size of 0.2 mm and 0.1 mm can provide consistent results in terms of accuracy and computational cost for quasi-static specimens and miniature dog-bone specimens,
Figure 5.2: Geometry of the specimens used for finite element analysis of (a) quasi-static (b) intermediate and high strain rate uniaxial tensile tests

respectively. Therefore, biased meshing, ranging from 0.5 mm at the grip section to 0.2 mm at the middle of the gauge length, was utilized for quasi-static simulation, and an element size of 0.1 mm was employed to discretize the gauge length of the miniature specimens. Rahmaan et al. \cite{68} indicated that DP600 does not exhibit noticeable anisotropic behaviour at each strain rate. Thus, isotropic behaviour based on the flow curve in the rolling direction was assumed in developing the VUMAT to reduce the complexity of simulations.

5.3.4 Material properties

The material, mechanical and damage parameters of the investigated DP600 are listed in Table 5.2. The material and plastic properties of the DP600 were obtained by carrying out uniaxial tensile tests at different strain rates. The tensile tests were also used to determine the Rousselier damage model, i.e. damage parameters ($D$ and $\sigma_1$). Determining $f_0$ is important for the integration of the Rousselier damage model
Table 5.2: Mechanical properties and damage parameters of the DP600

<table>
<thead>
<tr>
<th>$\sigma_y$ (MPa)</th>
<th>n</th>
<th>D</th>
<th>$\sigma_1$ (MPa)</th>
<th>$f_0$</th>
<th>$f_N$</th>
<th>$\varepsilon_N$</th>
<th>$S_N$</th>
<th>$f_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>340</td>
<td>0.148</td>
<td>2.5</td>
<td>425</td>
<td>0.0007</td>
<td>0.02</td>
<td>0.35</td>
<td>0.11</td>
<td>0.1</td>
</tr>
</tbody>
</table>

since this model is not able to predict any damage evolution if the initial void volume fraction is zero. The damage process in DP steels usually starts by the decohesion of martensite-ferrite interfaces or martensite cracking, depending on the martensite content of the alloy [3]. However, not all the martensite takes part in nucleating voids [23, 66]. Therefore, a fraction of the total volume content of martensite in the DP steels is considered as potential sites for void nucleation. In fact, the initial void volume fraction of this DP600 was experimentally measured to be 0.07% by Winkler et al. [71]

In order to determine the Rousselier damage parameters ($D$ and $\sigma_1$), uniaxial tensile tests were simulated at strain rates 0.1 and 1s$^{-1}$ using suggested hardening equations. Sarraf et al. [72] showed that the Rousselier model parameters do not have a significant effect on the predicted hardening behaviour but they can considerably change the onset and slope of the flow curve after maximum load is reached. Although fine tuning of the Rousselier parameters is required for each hardening function, the average values of $D$ and $\sigma_1$ were used as the initial Rousselier damage variables to avoid complications and simplify other parametric studies. These initial parameters are in very good agreement with the widely-used values for steel [73, 74]. Other damage parameters such as the strain controlled nucleation parameters and the final void volume fraction at failure ($f_f$) for DP600, used in this study, have been derived by several researchers using uniaxial tension tests and SEM analysis of the fractured specimens [2, 21, 23, 75]. These parameters are summarized in Table 5.2.
Table 5.3: Coefficients of hardening functions for DP600

<table>
<thead>
<tr>
<th>Hardening function</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>modified JC (mJC)</td>
<td>225.35</td>
<td>850.16</td>
<td>0.3194</td>
<td>0.0037</td>
<td>1.5715</td>
</tr>
<tr>
<td>Voce-modified JC (VmJC)</td>
<td>400.21</td>
<td>795.19</td>
<td>9.0236</td>
<td>0.0015</td>
<td>1.9430</td>
</tr>
<tr>
<td>KHL</td>
<td>161.54</td>
<td>946.48</td>
<td>0.2577</td>
<td>-0.1900</td>
<td>0.0037</td>
</tr>
</tbody>
</table>

5.4 Results and discussion

5.4.1 Hardening functions

In order to calculate the fitting parameters in the phenomenological constitutive equations shown in Eq. 5.2a-5.2c, a combination of non-linear regression (NLR) technique and Markov chain Monte Carlo (MCMC), as an optimization method, was used [72]. This new technique was employed to minimize the difference between experimental points obtained from the tensile tests and predicted values calculated by each hardening function. It has been shown that utilizing different optimization techniques can improve the result of the fitting procedure and lead to a considerable increase in the accuracy of the prediction made by a hardening equation [54]. The parameters in each hardening function were calculated for DP600 by the combined fitting procedure and are shown in Table 5.3.

Figure 5.3 shows the capability of each hardening equation to predict the uniaxial stress-strain curve of DP600 obtained at different strain rates. Comparing the experimental results and predicted curves, it can be understood that these three phenomenological hardening functions can accurately predict the flow behaviour of the investigated material in the range of studied strain rates considered. However, small differences can be observed near the yield point where the modified-JC and KHL underestimate the strength of the material at the beginning of plastic deformation. Also, they both over-predict the hardening rate compared with the experimental results at each strain rate. Nevertheless, it can be observed from Fig. 5.3 and 5.4 that there is very good agreement between the predicted and the experimental hardening curves of DP600 sheet at all strain rates.
Figure 5.3: Comparison of experimental flow stress curves of DP600 (dots)[68] with the fitted hardening equations (dashed lines) at different strain rates (0.001, 0.1, 1.0, 10, 100 s^{-1}) using (a) modified-JC (b) KHL and (c) Voce-modified JC models.
Figure 5.4: Comparison of experimental tensile strength and values predicted by constitutive equations at different strain rates for constant true strain values of 0.03, 0.06, 0.09, 0.12

5.4.2 Finite element simulation

Simulations of uniaxial tensile tests were carried out based on different test specimen geometries at strain rates ranging from 0.1 to 100 s\(^{-1}\). The simulations were used to study the effect of the hardening functions, void nucleation functions and void coalescence criteria on the performance of the Rousselier model in predicting the flow behaviour and damage evolution of DP600 sheets. It is worth noting that the figures in the following two Sections (Effect of void nucleation and Void coalescence criteria) were obtained based on the modified Rousselier damage model without any element deletion criterion. Also, the evolution of the Rousselier damage variable, the void volume fraction and the plastic limit load were derived from the centre of the gauge area.


Effect of void nucleation

Two of the most important parameters that need to be studied while evaluating the Rousselier damage model, are the damage variable and the void volume fraction. Figure 5.5 shows the history of the scalar damage variable ($\beta$) during the tensile deformation of the DP600 sheets at different strain rates. Results indicate a remarkable increase in the predicted damage variable when the void nucleation function is used as compared to the cluster nucleation condition where there is no nucleation of secondary voids. As it can be seen in Fig. 5.5, in both cases, the damage variable starts to increase from the beginning of the deformation but in the former case, due to the additional damage caused by the strain controlled void nucleation function, it increases at a much higher rate; e.g. the damage variable reaches $\beta = 4$ at $\varepsilon_{eq}^p = 0.2$, whereas $\beta < 1$ at the same strain level when $f_0$ remains constant. This trend is the same for all employed hardening functions. Moreover, the predicted damage growth is the same for different strain rates up to a strain level $\varepsilon_{eq}^p \simeq 0.2$ but beyond this, the damage growth rate decreases slightly in the quasi-static condition compared to other investigated strain rates. This can be attributed to the slightly different stress triaxiality (and its direct effect on the damage growth (Eq. 5.1c)) that elements experience due to the different geometries of quasi-static and miniature dog-bone specimens after the onset of localization, as shown in Fig. 5.6. Bardelcik et al. [76] and Rahmaan et al. [68] showed that the flow curves obtained from ASTM (E8M-04) and miniature tensile specimens are comparable up to the ultimate tensile stress, but after that their softening behaviour becomes different.

Another approach to assess the damage progress predicted by a micromechanical damage model is to evaluate the growth in void volume fraction since it can give a good indication of damage at different strain levels, strain rates and for different specimen geometries. The evolution of the void volume fraction ($f$) predicted by Rousselier damage model with and without the effect of secondary void nucleation is shown in Fig. 5.7. It can be seen that in all cases, the void volume fraction growth is negligible during the early stages of deformation. But after a certain strain level, approximately $\varepsilon_p = 0.3$ for strain controlled void nucleation and $\varepsilon_p = 0.8$ for the cluster
Figure 5.5: Evolution of scalar damage variable calculated by Rousselier damage model with (dashed lines) and without (solid lines) the effect of strain controlled void nucleation at different strain rates using (a) modified-JC and (b) Voce-modified JC hardening models.

Figure 5.6: Evolution of triaxiality as a function of equivalent plastic strain at strain-rates 0.1 and 100 $s^{-1}$ using (a) modified-JC and (b) Voce-modified JC.
nucleation condition, there is a rapid increase in the growth rate of the void volume fraction with subsequent linear increase in $f$ which can consequently lead to the final failure. The growth rate of the void volume fraction is approximately the same for different hardening functions and strain rates. Thus, it can be concluded that the evolution of the void volume fraction is somewhat independent of the hardening law and independent of strain rate for a given specimen geometry. However, it can be seen that utilizing a strain-controlled nucleation function causes the void volume growth to begin at much lower strains since the accumulation of nucleated voids increases the total void volume fraction ($df = df_g + df_N$) at each time increment during the simulation of the deformation process.

Figure 5.8 shows the engineering stress-strain curve of DP600 sheet obtained from experiments and predicted by the Rousselier damage model, with and without the effect of secondary void nucleation and using different hardening models. As it can be seen in Fig. 5.8, all predicted stress-strain curves are very similar up to a strain of $\varepsilon_p \leq 0.2$ for strain rates 0.1 and 100 s$^{-1}$. The reason for this is that the work hardening dominates the material behaviour even though the damage variable increases continuously. It can also be seen that the modified-JC and KHL hardening functions remarkably
overpredict the strain at which the onset of softening commences. However, employing a void nucleation function can significantly change this behaviour of unbounded hardening by introducing the secondary void nucleation as a mean of increasing the Rousselier damage variable at constant strain levels comparing with cluster nucleation condition, as shown in Fig. 5.5. The same effect can also be observed when a Voce-type hardening function is used where flow localization occurred at lower strain levels in case of utilizing the void nucleation function in the Rousselier damage model.

It should be noted that the second and third terms of the Rousselier plastic potential (Eq. 5.1b) are indicating the hardening and softening behaviour of the material, respectively. Therefore, using a nucleation function can help the softening term to overcome the second term at lower strain values. Moreover, considering the fundamental difference between Voce-type and power law-type hardening functions, the former demonstrates zero hardening rate after a certain stress level where the stress reaches a plateau. This makes it easier for the softening term in the damage model to dominate the flow behaviour and accelerate the damage process. Therefore, flow localization and failure occur at lower strain levels in Voce-type hardening functions comparing with modified Johnson-Cook and KHL.

It can also be seen from Fig. 5.8 that in the absence of a coalescence criterion, the model cannot predict the abrupt fracture at the end of the deformation process and therefore the predicted flow curve exhibits a continuous softening at high strain levels, which is obviously not consistent with experimental results. Accordingly, the Rousselier damage model requires an appropriate combination of a hardening function, controlled void nucleation function and void coalescence criterion in order to accurately predict the flow behaviour of materials from the beginning of the deformation process right up to the final fracture.

**Void coalescence criteria**

The performance of plastic limit load and the resultant coalescence criterion, proposed by Thomason [57, 59], can be assessed in different ways. On one hand, it can be calculated by Eq. 5.4 (hereafter referred as approach #1) and on the other hand, Eq. 5.7
Figure 5.8: Comparison of predicted flow curves by the Rousselier damage model and different hardening functions, with cluster nucleation (CN) and strain controlled void nucleation (SCVN) functions (dashed lines), with experiment (solid line) at strain rates (a) 0.1 (b) 100 s\(^{-1}\)
Figure 5.9: The effect of void nucleation function on the variation of plastic limit-load in the centre of tensile specimens for different hardening functions using $\alpha_t = f(n)$, at (a) 0.1 s$^{-1}$ and (b) 100 s$^{-1}$ calculated by approach #1 and approach #2, respectively. (CN: cluster nucleation, SCVN: strain controlled void nucleation function)

Figure 5.9 shows the evolution of normalized axial stress ($\sigma_I/\sigma_{eq}$) in the centre of the gauge area, predicted by the Rousselier model and different hardening models, as a function of the equivalent plastic strain for a strain rate of 0.1 s$^{-1}$ using approach #1 (Fig. 5.9a) and a strain rate of 100 s$^{-1}$ using approach #2 (Fig. 5.9b). In both cases, the predicted equivalent plastic strain at the onset of coalescence is too high when cluster nucleation is used in the model ($1.11 \leq \varepsilon_p \leq 1.16$ and $0.92 \leq \varepsilon_p \leq 0.95$) for approach #1 and #2, respectively. These values are very close to the fracture strains obtained from the experiments ($\varepsilon_f \simeq 1.0$) and predicted by phenomenological damage models ($\varepsilon_f \simeq 0.8$) and are therefore unrealistic. The onset of coalescence decreased significantly when strain controlled nucleation function was employed in the simulation where $0.483 \leq \varepsilon_p \leq 0.515$ for the two mentioned approaches. It is noteworthy that even though the coalescence plastic strains predicted using different hardening functions show a small deviation in case of Voce-modified JC comparing with other hardening models, the void nucleation function helps to reduce this difference to an insignificant value.
Figure 5.10: Variation of plastic limit-load in the centre of tensile specimens based on different approaches in calculating the ligament size ratio ($\chi$) at (a) 0.1 s$^{-1}$ using modified-JC hardening function and (b) 100 s$^{-1}$ using Voce-modified-JC hardening model

The evolution of the local strength, normalized to the homogeneous strength ($\sigma_I/\sigma_{eq}$) as a function of equivalent plastic strain using approach #1 and #2 and using constant and variable values of $\alpha_t$ is shown in Fig. 5.10. It can be seen that the localized strength predicted by approach #1 is too high at the beginning of the deformation while approach #2 predicts lower value although it is also still higher than what Benzerga [77] proposed in his research. However, comparing the results of constant and variable $\alpha_t$ employed in the model, reveals that using material hardening exponent can increase the plastic strain at the onset of coalescence. In another words, materials with greater ductility, and hence higher $n$ values, experience coalescence at higher strain levels. Also, it can be found that the critical strain value at the onset of coalescence predicted by the first approach is higher than that estimated by the second approach when cluster nucleation is used, but the former decreases significantly compared with the latter when a void nucleation function is employed.

Another way to analyse the performance of the coalescence criteria is to evaluate them based on the critical void volume fraction at the onset of coalescence ($f_c$) since each criterion predicts the point at which the localized deformation mode becomes equal to the homogeneous deformation mode differently. Figure 5.11 shows the evolution of the normalized axial stress as a function of the current void volume fraction at
Figure 5.11: Variation of plastic limit-load vs. current void volume fraction based on different hardening functions at strain rate $0.1 \text{ s}^{-1}$ with the effect of cluster void nucleation (CN) and strain controlled void nucleation (SCVN) calculated by (a) Eq. 5.4 (Approach #1) and $\alpha_t = \text{cte.}$, and (b) Eq. 5.7 (Approach #2) with $\alpha_t = f(n)$ strain rate $0.1 \text{ s}^{-1}$ using approach #1 (Eq. 5.4) and #2 (Eq. 5.7). As it can be observed from Fig. 5.11(a), under quasi-static conditions, the void nucleation function does not have a considerable effect on the prediction of $f_c$ when using the first approach, whereas it can significantly decrease the predicted value of $f_c$ when using the second approach. This exact pattern was also seen at strain rate $100 \text{ s}^{-1}$. Therefore, it can be concluded that Zhang’s approach (approach #1, Eq. 5.4) is less sensitive to the void nucleation process and hence, it is more consistent for predicting $f_c$. Evaluating all cases in Fig. 5.11, it can also be seen that predicting $f_c$ by the two mentioned approaches, with and without the void nucleation function, is practically independent of the hardening model that is used.

The plastic limit load evolution as a function of void volume fraction calculated by the first and second approaches and employing constant and variable $\alpha_t$ is shown in Fig. 5.12. It is calculated using the modified-JC and the Voce-modified JC hardening models at strain rate $0.1 \text{ s}^{-1}$. As it can be seen in Fig. 5.12(a,c), approach #1 predicted $f_c$ to be between 0.028-0.045 for the quasi-static. It is clear that the predicted critical void volume fraction at the onset of coalescence decreased by utilizing void nucleation function, yet increased by using $\alpha_t = f(n)$ instead of a constant $\alpha_t$. 

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Figure 5.12: Evolution of plastic limit-load vs. current void volume fraction based on modified JC at \( \dot{\varepsilon} = 0.1 \) s\(^{-1}\) using (a) Eq. 5.4 and (b) Eq. 5.7

However, approach #2 exhibited a different behaviour where employing a void nucleation function led to an increase in the estimation of \( f_c \). For this approach, the minimum \( f_c \) occurred when cluster nucleation was used such that it was predicted to be 0.021 at quasi-static strain rate, as shown in Fig. 5.12(b). Such behaviour is not normally expected. Comparing the results shown in Fig. 5.7 with the evolution of normalized axial stress in Fig. 5.9 reveals that although using a void nucleation function results in a significant decrease in the critical strain level at the onset of coalescence \( \varepsilon_c \) in both approaches, it cannot reduce \( \varepsilon_c \) enough for Approach #2 to reduce the value of \( f_c \) to the level predicted by the first approach.

### 5.4.3 X-ray tomography

X-Ray microtomography is one of the most effective ways to quantify the microstructure of materials or to analyse the damage and void evolutions in a ductile material [78]. In this study, SKYSCAN 1172-High Resolution Desktop Micro-CT at McMaster Automotive Research Centre (MARC), equipped with the Hamamatsu C9300 11Mpx camera, was used to investigate the porosity distribution in the tested DP600 sheets both qualitatively and quantitatively. Since the power was not sufficient for DP600 sheet material, Al+Cu filter was used to change the distribution of X-ray wavelength by decreasing the intensity of some special wavelengths from its spectrum within a
given beam. A rotational step of 0.4 ° was used in the test and the tomograph set-up was chosen to obtain the final image pixel size of 1.05 µm. Figure 5.13 shows the 3D representation of the fractured area on the miniature dog-bone specimens tested at 1 s⁻¹(a,b) and 100 s⁻¹(c,d). The geometry of the defused and localized neck as well as the dimensions of the investigated damaged area can be observed in Fig. 5.13(a,c). The distribution of the porosities are visible in Fig. 5.13(b,d) where the opacity of the matrix or region of interest (ROI) was reduced to 10% and made semi-transparent. It can be seen that the number of large voids near the fracture surface is slightly greater for the higher strain rate. As shown by Maire et al. [79], the accumulated damage visible in a 3-D X-ray tomography image appears to be more than expected since all cavities are exhibited in one view of the resulting 3-D rendering image. The actual fraction of porosities is less than what is expected from the image.
Figure 5.13: 3D representation of the necked area and accumulation of porosities in the miniature dog-bone specimens at strain rates (a,b) 1 s$^{-1}$ and (c,d) 100 s$^{-1}$.

The evolution of void volume fraction as a function of the distance to the fracture for different strain rates is shown in Fig. 5.14. Each point represents the closed porosity percentage on an image or slice of material perpendicular to the tensile loading direction. It can be clearly observed that the trend for both strain rates is the same: the void volume fraction remains low and nearly constant up to the localized neck, then it increases considerably in the local neck. This sudden increase can be attributed to the simultaneous void growth and cross-section area reduction. The
porosity percentage reaches approximately 2% close to the fractured surface.

Figure 5.14: Profile of the porosity percentage on the planes perpendicular to the load direction at strain rates (a) 1 s⁻¹ and (c) 100 s⁻¹

Despite some variations in the estimated $f_c$ by the combination of strain controlled void nucleation function and Approach #1 as well as the cluster void nucleation with Approach #2, the predicted ranges are in very good agreement with the results experimentally obtained in this study and the results published in the literature.

For instance, Maire et al. [79] measured void volume fraction at the centre of a miniature dog-bone shaped specimen using quasi-static in situ tensile tests. The X-Ray Tomography analysis of the specimens showed that $f_c$ = 2% before fracture. Also, numerical predictions from Butcher et al. [21] using numerical methods and those obtained by Abbasi et al. [80] conducting a comprehensive fitting procedure, showed the same values for $f_c$.

### 5.4.4 Performance of the modified damage model

The effect of controlled void nucleation function combined with void coalescence criteria on the engineering flow curve of DP600 sheet predicted by Rousselier damage model using different hardening functions at strain rates 0.1 and 100 s⁻¹ is shown in Fig. 5.15.

It can be seen that the post coalescence behaviour of predicted flow curves is improved significantly and the modified model demonstrates the sudden failure at onset of
fracture. Moreover, no difference can be detected between the predicted flow curves derived when the Zhang or Chambert approaches are used to establish the coalescence criterion. Although they calculated the parameters of Thomason’s plastic limit load criterion differently, the overall macro-scale material response predicted similar results with both approaches.

However, the predicted fracture strain is slightly over-predicted when using KHL and modified-JC hardening models, even with the void nucleation function, and it is underestimated when using a Voce-type hardening function. It is worth noting that the average value of $\sigma_1$ and $D$ was used, as mentioned in Section 5.3.4. Accordingly, re-calculation of Rousselier damage function parameters ($\sigma_1$ and $D$) is necessary for both power law- and Voce-type hardening models in order to obtain accurate flow curves at different strain rates.

Figure 5.15: Predicted flow curve of DP600 sheet using Rousselier damage model combined with strain controlled void nucleation function and void coalescence criteria at (a) $\dot{\varepsilon} = 0.1 \text{ s}^{-1}$ using KHL model and (b) $\dot{\varepsilon} = 100 \text{ s}^{-1}$ using Voce-modified JC model

The result of fine tuning the modified Rousselier model, i.e. the original damage model combined with void nucleation function, a void coalescence criterion and a void growth acceleration function, is shown in Fig. 5.16. For both types of hardening models, $D = 2$ was obtained as the first parameter, and $\sigma_1 = 435$ and 480 (MPa) were determined for power law- and Voce-type models, respectively. The difference between the values of $\sigma_1$ for different hardening models is decreased considerably by using the strain controlled...
void nucleation function and coalescence criterion, compared to the values initially calculated by Sarraf et al. [72] using the original Rousselier damage model. Zangeneh et al. [32] showed that $\sigma_1$ and $D$ are not transferable between different triaxiality levels. However, despite the fact that the triaxiality of both specimen geometries are the same during uniform deformation and diverge during post-uniform deformation (as shown in Fig. 5.6), the difference between the damage parameters for both specimen geometries was negligible.

Figure 5.16: Comparison of experimental results and simulation results predicted by re-determined Rousselier damage model using void nucleation function and Thomason-Zhang void coalescence criterion

The distribution of the accumulative damage variable across the tensile specimens as predicted by the Rousselier damage model, using different hardening and void nucleation functions, is shown in Fig. 5.17. These distributions were determined when the maximum load was reached and diffuse necking was initiated at strain rates 0.1 and 100 s$^{-1}$. In all cases, strain localization initiated in the centre of the gauge area and all specimens experienced diffuse necking, however, damage is more localized on the shear bands when the Voce-modified JC hardening function was used in the Rousselier model.
at $\dot{\varepsilon} = 0.1 \text{ s}^{-1}$. It can be attributed to the behaviour of saturation hardening functions where the hardening rate becomes zero at high strain levels. An important point is that the maximum $\beta$ in the centre of the diffuse neck was predicted to be approximately 3.3 and 3 for strain rates 0.1 and 100 s$^{-1}$ respectively when cluster nucleation was employed, which indicates that the material in the neck should accommodate a considerable amount of strain during non-uniform deformation to reach the critical scalar damage variable at failure. On the contrary, using a strain controlled void nucleation function leads to an increase in the overall damage accumulation in the gauge area and specially in the neck, and consequently the non-uniform plastic deformation decreases which accelerates the failure process. Nonetheless, the distribution of $\beta$ and the geometry of the localization become somewhat similar for both types of hardening models when strain controlled void nucleation is employed, as shown in Fig. 5.17a. Therefore, it can be concluded that the dependency of the accumulative damage distribution on the hardening model after the onset of necking is reduced in the modified Rousselier model where a strain controlled void nucleation function is utilized.
Figure 5.17: Distribution of the damage accumulation at the onset of necking using different hardening models and void nucleation functions at (a) 0.1 and (b) 10 and (c) 100 s$^{-1}$.

The effect of hardening models, void nucleation functions and void coalescence criteria on the distribution and geometry of damage along the gauge of tensile specimens, tested at 0.1, 10 and 100 s$^{-1}$, is presented in Fig. 5.18. Similar to the experiments, it can
be seen that the predicted localization and failure begin from the centre of specimens in all strain rates where eventually, the fully damaged elements are removed from the FE models. It has been shown that the intensity of strain localization on shear bands in quasi-static specimens is not sufficient to predict the failure on either of them when using unbounded-hardening models and the cluster nucleation function \[72\]. It is also shown that the damage front propagates from the centre of the gauge towards the edge of specimens (perpendicular to the tensile axis) when unbounded-type hardening models (eg. the KHL and modified-JC) are used to describe the flow behaviour of materials in the Rousselier damage model. But the final failure would occur on shear-bands when using Voce-type models. Nevertheless, using a strain controlled nucleation function and void coalescence criterion can reduce the dependency of the Rousselier damage model on the hardening function and improve its performance to predict the final geometry of failure in quasi-static specimens where the accumulation of damage would be significantly intensified on shear bands. Therefore, the dominant mechanism becomes localized necking and fracture on the shear bands for all hardening models utilized, which is in good agreement with what has been observed in the experiments and is shown in Fig. 5.18a. It should be noted that using the full-geometry instead of a quarter-geometry would result in damage localization on shear bands in an X-shape which causes the final failure to take place along either of the shear bands.

It can be observed from Fig. 5.18(b,c) that in all models, the damage is predicted to commence at the centre of specimens deformed at 10 and 100 s\(^{-1}\) and to propagate radially outward across the cross section of the gauge area of the tensile specimens. Although the predicted fracture geometries are somehow similar between various simulation conditions, the damage accumulation and distribution are considerably different at each strain rate when the strain controlled void nucleation and void coalescence criteria are utilized compared to the original Rousselier damage model with cluster nucleation. The former combination of the Rousselier damage model and complementary functions predicted the damage accumulation to be more uniformly distributed along the gauge area which results in smaller post-uniform deformation and a shorter diffused-neck, which is in good agreement with the experiments. In addition, the performance of the Rousselier model in predicting the distribution of \(\beta\)
and the final damage geometry becomes independent of the hardening function by employing a strain controlled void nucleation function and a void coalescence criterion.

Figure 5.18: Experimental and predicted damage accumulation and damage geometry at (a) 0.1 and (b) 10 and (c) 100 s\(^{-1}\) using different hardening functions, void nucleation functions and a void coalescence criterion (approach #1: Eq. [5.4])

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5.5 Conclusions

The uniaxial flow behaviour and damage evolution of DP600 sheets were studied at different strain rates, ranging from quasi-static conditions (0.001s\(^{-1}\)) to high strain-rates (100s\(^{-1}\)). In this study, different hardening models, different void nucleation functions as well as void coalescence criteria were successfully implemented in the Rousselier ductile damage model.

The original Rousselier model is not capable of predicting the sudden failure at the end of the deformation process. In addition, the cluster nucleation function assumed in the original Rousselier model does not take the effect of secondary void nucleation into account. Therefore, the critical strain at the onset of coalescence and final fracture is overestimated. It was found that employing a strain controlled nucleation function can significantly improve the ability of the Rousselier model to predict these critical strains.

Furthermore, two approaches were used to calculate the evolution of the void space ratio parameter in Thomason’s plastic limit load coalescence criterion. It was shown that the performance of both models is the same at the macro-scale but at the element-scale, their behaviours are slightly different. Both models demonstrated acceptable results in terms of determining the critical void volume fraction at the onset of coalescence. They are in good agreement with the experimental values measured in this study via X-Ray tomography and those reported in the literature for DP600 tensile specimens, although approach #1 (Eq. 5.4) showed a more stable behaviour for a range of conditions.

Utilizing complementary functions such as a void nucleation function, a void coalescence criterion and post-coalescence treatment can significantly improve the performance of the Rousselier damage model in predicting the damage behaviour, the distribution of damage accumulation along the gauge area, and final damage geometry to become independent of the hardening model. However, it is necessary to calibrate the parameters in the Rousselier damage model for each hardening function in order to obtain accurate flow curves. Nevertheless, the wide range of \(\sigma_1\) values obtained by using the original Rousselier model with power law-type and Voce-type hardening models, is
significantly decreased by using these complementary functions and criteria.

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5.6 Bibliography


Chapter 6

Numerical analysis of damage evolution and formability of DP600 sheet with an extended Rousselier damage model

This chapter describes Marciniak formability tests carried out to determine the forming limit curve (FLC) of DP600 steel sheet, and an extended version of Rousselier’s ductile damage model, which accounts for void nucleation, growth and coalescence was used to simulate the tests and predict strain localization and failure for three different strain paths: uniaxial tension, plane strain and biaxial tension. In addition, a combination of flat rolling and uniaxial tension tests were used to generate the extended flow curve of the material. Damage evolution in terms of Rousselier scalar damage variable and void volume fraction was assessed for each simulation condition. The FLC as well as neck and fracture morphologies and geometries were obtained from finite element simulations of the Marciniak tests and compared to experimental results. The sensitivity and dependency of the predicted necking limits, damage distribution and geometry predicted by the Rousselier damage model to the type of hardening model, strain path, void nucleation function and void coalescence criterion are discussed. The modified Rousselier model was shown to successfully predict the FLC, damage distribution and the final damage geometry of DP600 sheets.
6.1 Introduction

Numerical determination of sheet metal formability as well as the onset of strain localization, instability and failure is of interest in both academia and sheet metal forming industry. A quantitative prediction of the limiting strain requires precise and comprehensive assessment of both necking and failure especially for new grades of sheet metals that show high strength along with high ductility and excellent weight-to-strength ratio, such as dual-phase (DP) and transformation induced plasticity (TRIP) steels. DP steels offer very good mechanical and forming properties due to their combined strength, ductility and high work hardening rate. The properties of DP steels are a result of their microstructure where hard martensite is dispersed throughout the ductile ferrite matrix. Therefore, they have become one of the most widely-used sheet metals in the automotive industry and efforts continue to be made to reduce the weight, increase the strength and safety, and decrease the production cost of DP automotive parts. To evaluate the forming behaviour of DP600 steel, researchers have examined the strain path and strain rate dependency of the formability of DP600 in a cross-die test, in tube hydroforming, tube hydropiercing, and electrolydraulic free-forming and die–forming. Accordingly, reliable experimental test data are required in order to evaluate the formability of the sheet material and to develop accurate numerical models to predict its behaviour and structural integrity.

The strain level that a material can reach without experiencing any instability or localization is considered to be its forming limit and strongly depends on the strain path the sheet material experiences. Keeler and Backofen, and Goodwin were the first to propose the concept of a forming limit curve (FLC) in principal strain space. They proposed to determine the FLC by measuring the major and minor strains in the sheet plane at the onset of strain localization for a wide range of strain paths from uniaxial tension to equi-biaxial tension. In other words, local plastic instability is the deformation limit of sheet metal under plane stress forming conditions and can usually be described by a forming limit diagram (FLD). Two of the most widely-used approaches to assess the formability of a material are the Nakazima test as an out-of-plane stretching test (hemispherical punch) and the...
Marciniak test as an in-plane stretching test (flat bottom punch) [17][18]. These tests are carried out by deforming the sheet metal along different strain paths up to the onset of necking. Afterwards, a grid analysis technique is used to measure strains in the necks and these are used to generate the FLC. The normal loading, bending and non-uniform strain distribution in the Nakazima tests make interpretation of the forming limit data somewhat complicated. In contrast, the Marciniak test utilizes a carrier blank between the flat-bottom punch and the sheet metal specimen and therefore leads to proportional strain data results without the effects of bending or friction [16][19]. Since computational techniques such as the finite element method (FEM) have become widely-used, researchers have employed these techniques to simulate these formability tests and numerically analyse the formability of materials and predict the FLCs: Zadpoor et al. [20] employed commercial finite element simulation software to simulate the limiting dome height (LDH) test and used Storen-Rice analysis to increase the accuracy of the limiting strains. Pepelnjak and Kuzman [19] proposed a computational method to determine the localization and generate the FLC for a low carbon steel. Mahboubkhah [14] evaluated the uncertainty of four different strain measurement methods to analyse the limiting strains in St13. Simha et al. [13] presented a comprehensive method to obtain stress-based and extended stress-based forming limit curves of 5xxx series aluminium alloys. Ramazani et al. [3] employed the Gurson-Tvergaard-Needleman (GTN) [21][22] damage model to predict the formability of DP600 in a cross-die test. Abbasi et al. [23] used the same damage model to simulate the LDH test of tailor-welded blanks (TWBs) and calculate their FLC. Kolasangiani et al. [24] used a combination of FEM and the Cockcroft and Latham ductile fracture criterion [25] to simulate the Erichsen test and generate the FLC of SS304L steel sheet. Maris et al. [26] simulated and compared the FLCs obtained from quasi-static Marciniak tests and those achieved from high-strain rate electro-hydraulic forming of DP600 and AA5182 sheets. It can be seen that an appropriate ductile damage model, work hardening function, void nucleation function and void coalescence criteria can be implemented into a numerical code to increase the accuracy of simulation results since different combinations of models and functions can significantly affect the final results [27].
The Rousselier ductile damage model [28] is a widely-employed micro-scale model for predicting ductile fracture. The Rousselier model requires fewer constants to be defined compared to the well-known Gurson–Tvergaard–Needleman [22,29] damage model and it has the capability of predicting damage evolution and void volume fraction growth at very low, zero or negative stress triaxiality. Furthermore, unlike the GTN model which defines the damage evolution in a material based on the growth of a spherical or cylindrical shaped void, the Rousselier damage model was developed without consideration of the shape of voids and accordingly, it can determine the damage transition from flat to oblique fracture surfaces [30,31]. The Rousselier damage model was used by Besson et al. [32] to model crack growth and to show that cup-cone fracture formation could be better predicted by using this model compared to GTN damage model. In addition, he investigated the effect of different parameters such as mesh size on the performance of the Rousselier model in predicting oblique fracture [32]. It has also been used by Poussard et al. [33] to simulate smooth tensile and compact tension specimens, and Tu et al. [34,35] employed it to evaluate the ductile damage and crack growth on S355NL steel electron beam welded joints and aluminium laser-welded joints. Nevertheless, although the initial void volume fraction is required in the Rousselier model, no secondary void nucleation function or void coalescence criterion was defined in this model. Zanganeh et al. [36] proposed an approach to couple the Rousselier model with Thomason’s plastic limit load coalescence criterion [37,38] to model the damage and fracture behaviour in uniaxial tension of AA2050 with different positive triaxiality levels using notched specimens. Having considered the advantages and capabilities of the Rousselier damage model, it was used to evaluate the formability, damage and fracture behaviour of DP600 steel sheets deformed in quasi-static Marciniak formability tests.

In this study, DP600 steel sheets were deformed along different strain paths, and strain measurements were carried out to generate the experimental FLC. Furthermore, finite element modelling was used to simulate the Marciniak tests for three strain paths: uniaxial tension (UT), plane strain (PS) and biaxial tension (BT) and predict the FLC. In order to define the flow hardening of the DP600 sheet, a series of flat rolling experiments followed by uniaxial tension tests were employed to obtain the extended
hardening curve of the material up to large strains. Subsequently, two different types of hardening models, saturated and unbounded types, were fitted to the experimental flow curves. In addition, various void nucleation functions, a void coalescence criterion and a void growth acceleration function were implemented in the Rousselier damage model to make it as complete and as accurate as possible. Accordingly, this extended damage model was implemented in a user material subroutine (VUMAT) framework that was used in ABAQUS/Explicit finite element simulation software. A comprehensive study was then performed to evaluate the effect of hardening function types, void nucleation models and void coalescence criteria on the damage evolution, instability and localization, and damage and fracture geometry of the Marciniak test specimens. The numerically predicted FLC is then compared to the experimental one and the performance of the extended Rousselier damage model in predicting the limiting strains as well as the neck and fracture morphologies are discussed.

6.2 Constitutive modelling of ductile fracture

6.2.1 Micromechanical damage model

In modern damage mechanics, failure of a ductile material is described by micromechanical damage models using nucleation, growth and coalescence of micro-voids. In this regards, void volume fraction is usually considered as the damage parameter \[ \Phi \]. The most important continuous ductile damage models were developed by Rice and Tracey \[40\], Tvergaard and Needleman \[22\] and Rousselier \[28\]. Both GTN and Rousselier are thermodynamically consistent ductile damage theories where the former was developed based on thermodynamic considerations while the latter was developed based on the porous material concept and description \[32\]. Rousselier \[28,41\] proposed a plastic potential based on the decomposition of the free Helmholtz potential energy (\(\Phi\)) into stored elastic (\(\Phi_e\)), plastic (\(\Phi_p\)) and damage energy (\(\Phi_d\)) \[30,39\] :

\[
\Phi(\varepsilon_e, \varepsilon_p, f) = \Phi_e(\varepsilon_e) + \Phi_p(\varepsilon_p) + \Phi_d(f)
\] (6.1a)
where $\varepsilon_e$, $\varepsilon_p$ and $f$ are the elastic strain, plastic strain and the void volume fraction, respectively. The Rousselier constitutive damage model \cite{41}, as an isotropic–hardening and isotropic–damage, modifies the plastic potential or yield surface and is written as

$$
\Phi = \frac{\sigma_{eq}}{(1-f)} - H(\varepsilon_p) + B(\beta)D \exp \left( \frac{\sigma_m}{(1-f)\sigma_k} \right) = 0 \quad (6.1b)
$$

where $\sigma_{eq}$ is the von Mises equivalent stress, $\sigma_m$ denotes the hydrostatic stress, and $B(\beta)$ is a damage function and is the conjugate force to the scalar damage variable ($\beta$). In the Rousselier damage model, the constants that describe the resistance of the material to damage growth and coalescence are $D$ and $\sigma_k$. The true stress-true plastic strain hardening behaviour of the material is defined by $H(\varepsilon_p)$. The damage parameter ($\beta$) is defined as a function of the plastic multiplier in the normality rule ($\lambda$) or plastic strain increment ($\dot{\varepsilon}_p$). The evolution function of $\beta$ is given by

$$
\dot{\varepsilon}_p = \lambda, \quad \dot{\beta} = \dot{\varepsilon}_pD \exp \left( \frac{\sigma_m}{(1-f)\sigma_k} \right) \quad (6.1c)
$$

The original Rousselier damage model predicts the evolution of damage based on an initial void volume fraction ($f(0) = f_0$) and void growth rate, hence no void nucleation function is considered in this model, i.e. $df = df_g$. In the absence of an initial void volume fraction, the Rousselier model is not able to predict any damage progress and will be equal to von Mises yield criterion. The current void volume fraction can be determined based on the damage function, scalar damage variable and initial void volume fraction ($f_0$).

$$
f = \frac{B(\beta)}{\sigma_k} = \frac{f_0 \exp(\beta)}{1 - f_0 + f_0 \exp(\beta)} \quad (6.2a)
$$

Using phenomenological plastic hardening models is a well-known approach to define the true stress-strain curve of different materials \cite{42}. These hardening models can be described as “saturated” when the strain hardening of the material reaches a saturation stress at large strains and as “unbounded” when there is no limit of strain hardening at high strains \cite{43}. Three different rate-independent isotropic hardening models were
used to model the plastic behaviour of the DP600 sheet: (1) Ludwik’s law \[44, 45\] as a power hardening law where the hardening rate \((d\sigma/d\varepsilon)\) is non-linear at large strains (Eq. 6.3a), (2) the 3-parameter Voce model \[46\] as the main saturated-type model (Eq. 6.3b), and (3) the 4-parameter Voce model (Eq. 6.3c) which takes stage IV hardening of materials into account as a linear function of plastic strain \[47, 48\].

\[\begin{align*}
H(\varepsilon_p) &= C_1 + C_2 \varepsilon_p^{C_3} & (6.3a) \\
H(\varepsilon_p) &= C_1 - (C_1 - C_2) (1 - \exp(-C_3\varepsilon_p)) & (6.3b) \\
H(\varepsilon_p) &= C_1 - (C_1 - C_2) (1 - \exp(-C_3\varepsilon_p)) + C_4 \varepsilon_p & (6.3c)
\end{align*}\]

In equations 6.3a-6.3c, \(C_{1...n}\) are the material constants and \(\varepsilon_p\) represents the equivalent plastic strain.

### 6.2.2 Void nucleation function

Rousselier \[41\] adopted a cluster nucleation function \((f_0 = \text{cte.})\) for his damage model, in which there is no secondary void nucleation, to predict the damage evolution. Several researchers \[3, 6, 49, 50\] have shown that DP steels and TRIP steels exhibit secondary void nucleation throughout the deformation up to the final failure. Various void nucleation functions have been proposed in the literature such as continuous nucleation \((df_N/d\varepsilon_p = A_0)\) \[38\] which has been used to model the damage of aluminium \[36, 51\] and steel \[52\]. However, Chu and Needleman \[21\] proposed that the void nucleation may be controlled by a normal distribution function based on strain \((A\,d\varepsilon_p)\), stress \((B\,d\sigma_{eq})\), or hydrostatic stress \((C\,d\sigma_m)\) \[53\]. Since strain-controlled void nucleation, Eq. 6.4 has been shown to be the most appropriate secondary void nucleation function for DP600 due to its mean size of martensite particles \[2, 3, 6\], this function was used in this study to include void nucleation into the Rousselier damage model.
\[ df_n = A \, d\varepsilon_p + B \, d\sigma_{eq} + C \, d\sigma_m \]  
\[ A = \frac{f_N}{S_N \sqrt{2\pi}} \, \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{S_N} \right)^2 \right] \]  
\[ B = C = 0 \]

In Eq. 6.4(a,b), \( df_n \) represents the void nucleation rate, \( f_N \), \( \varepsilon_N \) and \( S_N \) are the volume fraction of void nucleating particles, the mean value and the standard deviation of the normal distribution of nucleating strain, respectively.

### 6.2.3 Void coalescence criterion and post coalescence regime

In the final stages of failure, the deformation localizes and the strength of the material decreases rapidly due to the linkage of voids and formation of microcracks. Therefore, coalescence can be described as the transference of homogeneous deformation mode to a severe localized mode between voids [54]. In the GTN damage model, the critical void volume fraction at the onset of coalescence (\( f_c \)) is considered to be constant [22], however, it is shown that \( f_c \) is strongly dependent on the initial void volume fraction, the strain path [6, 38], and the stress state [36].

In this regard, the plastic limit load (PLL) criterion proposed by Thomason [37, 55] has become one of the most widely-used models to model coalescence numerically. The PLL model has defined coalescence as a function of the necking of the ligament between voids. Thomason stated that the stress needed for the homogeneous deformation mode is considerably lower than that needed for the localized deformation mode. As the deformation progresses, the localized strength decreases due to the increase in void volume fraction until it becomes equal to the stress required for homogeneous deformation in which coalescence happens. The void volume fraction at that point can be considered as the critical value for the onset of coalescence. Several researchers proposed various extensions to Thomason’s model to calculate different parameters of this model [38, 56], taking the void shape [57] or cell geometry and mechanical
properties \([58, 59]\) into account. The plastic limit load criterion proposed by Zhang et al. \([38]\) is written as follows:

\[
\frac{\sigma_I}{\sigma_{eq}} = \left[ \alpha_t \left( \frac{1}{\chi} - 1 \right) + \frac{\beta_t}{\sqrt{\chi}} \right] (1 - \pi \chi^2) \tag{6.5a}
\]

\[
\chi = \left( \frac{3f}{4\pi} \exp(\varepsilon_I + \varepsilon_{II} + \varepsilon_{III}) \right)^{1/3} \left( \frac{(\exp(\varepsilon_{II} + \varepsilon_{III}))^{1/2}}{2} \right)^{-1} \tag{6.5b}
\]

where \(\sigma_I\) is the maximum principal stress, \(\alpha_t\) and \(\beta_t\) are model constants, \(\chi\) represents the void space ratio, and \(\varepsilon_{I,II,III}\) denote principal strains. It has been shown by Pardoen and Hutchinson \([58, 59]\) that the prediction of the model would be improved if the first model constant \((\alpha_t)\) is expressed as a function of the strain hardening exponent \((n)\) in a power law hardening model: \(\alpha_t = 0.1 + 0.217n + 4.83n^2\) for materials with \(0 \leq n \leq 0.3\), and \(\beta_t \simeq 1.24\).

After void growth and the onset of coalescence at \(f_c\), the load bearing capacity of the material decreases sharply to the final failure. Tvergaard and Needleman \([22]\) suggested a void volume acceleration function to take the effective porosity \((f^*)\) into account during the post-coalescence regime. Complete loss of material strength and load carrying capacity occurs when the void volume fraction reaches its critical value at the time of total failure \(f_F\). The effective void volume fraction is given by:

\[
f^* = \begin{cases} 
  f & \text{if } f \leq f_c \\
  f_c + \frac{f_u^* - f_c}{f_F - f_c} (f - f_c) & \text{if } f \geq f_c 
\end{cases} \tag{6.6}
\]

where \(f_u^*\) is the final effective void volume fraction at final failure (when \(f = f_F\)). As it can be seen in Eq. \([6.6]\), the rate of void growth acceleration is also a function of \(f_F\) which implies that a lower void volume fraction at failure leads to faster void growth acceleration and thus, faster loss of load bearing capacity of the material.
6.3 Material and methods

6.3.1 Material properties

The material studied in this research was a DP600 steel sheet with a nominal thickness of 1.48 mm. The chemical composition of as-received DP600 sheet is given in Table 6.1. The elastic properties of the DP600 were derived from Butcher et al. [6] and uniaxial tensile tests were employed to obtain the mechanical properties of the as-received material, which are shown in Table 6.2.

Table 6.1: Chemical composition of the material (wt%) [10]

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>Cr</th>
<th>Mo</th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.107</td>
<td>1.5</td>
<td>0.18</td>
<td>0.18</td>
<td>0.21</td>
<td>0.06</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Table 6.2: Mechanical properties of as-received DP600 sheet

<table>
<thead>
<tr>
<th>Parameters</th>
<th>$E$ [GPa]</th>
<th>$\nu$ [6]</th>
<th>$\rho$ [kg/m$^3$]</th>
<th>$\sigma_y$ [MPa]</th>
<th>$\sigma_{UTS}$ [MPa]</th>
<th>$\varepsilon_{UTS}$ [%]</th>
<th>$\varepsilon_t$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values</td>
<td>206</td>
<td>0.3</td>
<td>7800</td>
<td>375</td>
<td>617</td>
<td>17.4</td>
<td>25.5</td>
</tr>
</tbody>
</table>

In addition to the elastic-plastic mechanical properties of the investigated DP600 sheet, correct determination of the damage parameters such as the Rousselier damage model parameters, i.e. $D$ and $\sigma_k$, initial void volume fraction and void nucleation function parameters is essential for modelling ductile damage. One of the widely-used approaches to correctly identify damage model parameters is the inverse method [23, 60] which consists of finding the best fit between the flow curve generated by the finite element simulation, and the experimental tensile data. The fitting parameters which obtain the best fit between simulations and experiments, are considered as the damage model parameters. Sarraf et al. [61] explicitly described the calibration procedure of $D$ and $\sigma_k$ for the Rousselier damage model. It has also been shown that altering $D$ and $\sigma_k$ does not lead to a considerable change of the predicted hardening...
behaviour in the uniform deformation, but they effectively determine the onset and
the slope of the flow curve after maximum load is reached \[36, 61\]. In this study,
\(D=2.5\) and \(\sigma_k=425 \text{ MPa}\) were found to be the material constants in the Rousselier
damage model for this DP600 steel and are in good agreement with the widely-used
values for steel \[34, 61, 62\]. Although calibrating the Rousselier damage model based
on each strain path can lead to more accurate predictions, constant parameters were
determined in order to evaluate the accuracy of the proposed model in predicting the
FLC of DP600 specimens and simplifying the parametric study.

Unlike the GTN model, the Rousselier damage model is unable to predict any damage
evolution in the absence of an initial void volume fraction. Therefore, \(f_0\) should be
specified at the beginning of the simulation. It has been shown that the onset of
the damage is a result of the decohesion of martensite-ferrite interfaces or martensite
cracking, depending on the martensite content of the steel \[5\]. Since not all of the
martensite in a DP steel participates in the void nucleation process \[2, 10\], only
a fraction of the volume content of martensite is determined as possible sites for
nucleation of the initial voids. Winkler et al. \[63\] experimentally determined the initial
porosity of DP600 to be 0.07% and this value was used in the Rousselier damage model
to set \(f_0\). Different researchers derived the strain-controlled nucleation parameters
such as the volume fraction of void nucleating particles and nucleation strain, as well
as the final void volume fraction at failure \((f_F)\) either by utilizing uniaxial tension tests
or SEM analysis of the fractured specimens \[2, 3, 6, 64\]. Table \ref{tab:6.3} shows a summary
of these parameters. It is worth mentioning that the void volume fraction at the onset
of coalescence is not pre-determined in this model since the coalescence criterion was
used as a controlling function.

\begin{table}[h]
\centering
\caption{Rousselier damage parameters for DP600 \[2, 3, 6, 63\]}
\begin{tabular}{cccccccc}
\hline
\(\bar{D}\) & \(\sigma_k \text{ (MPa)}\) & \(f_0\) & \(f_N\) & \(\varepsilon_N\) & \(S_N\) & \(f_F\) \\
\hline
2.5 & 425 & 0.0007 & 0.02 & 0.35 & 0.11 & 0.1 \\
\hline
\end{tabular}
\end{table}

180
6.3.2 Uniaxial tensile tests

Uniaxial tensile tests were performed on DP600 sheets using a MTS Model 43 Universal testing machine with a 50kN load cell. In this work, ASTM E8M tensile specimens, as shown in Fig. 6.1, were first machined from previously sheared strips using wire electric discharge machining (EDM) and then tested at a low strain rate of 0.001 s\(^{-1}\). To obtain this strain rate, a cross-head velocity of 0.083 mm/s was used under displacement control. Prior to running the tests, a speckle pattern was applied to the tensile specimens for image based strain measurements using Digital Image Correlation (DIC) techniques. To use the DIC method, the specimens were first painted in white followed by the application of a stochastic black speckle pattern that deforms with the specimen during the test. A ±25 mm biaxial extensometer was utilized to measure the axial and width strains. Additionally, video extensometer and DIC post processing software along with 25 mm camera lenses with 25 Hz sampling rate were used for strain measurements. The data points obtained from the MTS machine, biaxial extensometer and DIC cameras were subsequently synchronized in a custom built code developed in MATLAB environment for further post processing and data analysis. Consequently, engineering stress was obtained by dividing the measured load by the initial cross-sectional area of the gauge, and then used to calculate the true-stress. DIC measurements were used to directly obtain the true-strain. The experimental true stress-true strain curve was employed to fit the hardening functions.

![Figure 6.1: Geometry of the uniaxial tension specimen (ASTM E8M)](image)
6.3.3 Uniaxial tensile tests combined with incremental rolling

The hardening curve is an important mechanical characteristic that needs to be provided for finite element simulation. One of the main limitations of a traditional uniaxial tensile test is that it only provides the true-stress true-plastic strain flow curve of materials up to a certain strain level, usually just over 0.2 for typical low carbon steel grades, and much lower for some AHSS grades [65, 66]. A usual way to deal with this problem in a FEM simulation is to extrapolate the flow curve beyond the ultimate tensile strength, but this can introduce some errors in the simulation. Since sheet metals can undergo greater levels of deformation in the stamping process due to biaxial stress states, it is necessary to conduct a mechanical test that can demonstrate the material’s response at high strain. Various tests such as the uniaxial compression test, hydraulic bulge test, viscous pressure bulge test and shear test can be employed to determine the large-strain flow stress of materials.

Ford [67] and Hecker et al. [68] proposed a method to extend the flow curve of the material obtained in uniaxial tension to higher strain levels by including a compressive pre-strain generated by flat rolling of the sheet material prior to the tensile test. Sevillano et al. [69] have shown that the flat rolling of sheet metals induces homogeneous deformation and therefore, is one of the best processes for pre-straining the material to large strain levels. Despite the possible discrepancy in the flow curve caused by the change in the deformation mode, this method provides experimental data that extend the flow curve up to strains greater than 1.0, which is much more reliable than extrapolating the tensile data of the as-received material. This method was employed by different researchers to obtain the forming behaviour of AA1200 alloy [70] and DP600 [71] beyond the limits of standard ASTM E8/E8M (2008) tensile tests. Although isotropic hardening is an acceptable assumption for forming processes in which the sheet metal undergoes somewhat linear loading strain paths, kinematic hardening effect as a result of stress reversal or stress state change should be considered [72]. However, isotropic hardening was assumed in this research and the implementation of kinematic hardening is left for future work.
The procedure for performing tensile tests after successive increments of rolling was the same as for standard tension tests. Nevertheless, various levels of pre-strain were induced by rolling prior to the tensile loading and subsequently added into the total strain. To determine the pre-strain values, electro-etching on sheet metal strips was performed to create a 2.5 mm square grid, as shown in Fig. 6.2. Actual effective plastic pre-strains were obtained by analysing the change in grid length and width. For each pre-strain value, two tensile tests were carried out to confirm the repeatability and consistency of the results. Details of sample designation, thickness and pre-strain data are provided in Table 6.4. Subsequent to the pre-straining, ASTM E8 tensile specimens were then machined from the rolled strips using wire electric discharge machining (EDM). Following that, speckle patterns were applied to tensile specimens for image-based strain measurements, as shown in Fig. 6.2.

Table 6.4: Description of specimens pre-strained by flat rolling

<table>
<thead>
<tr>
<th>SD</th>
<th>$t_t$(mm)</th>
<th>$\varepsilon_t$</th>
<th>$t_x$(mm)</th>
<th>$\varepsilon_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SR1-1</td>
<td>1.483</td>
<td>0.0</td>
<td>1.483</td>
<td>0.0</td>
</tr>
<tr>
<td>SR1-2</td>
<td>1.493</td>
<td>0.0</td>
<td>1.493</td>
<td>0.0</td>
</tr>
<tr>
<td>SR2-1</td>
<td>1.256</td>
<td>0.2</td>
<td>1.262</td>
<td>0.193</td>
</tr>
<tr>
<td>SR2-2</td>
<td>1.255</td>
<td>0.2</td>
<td>1.259</td>
<td>0.196</td>
</tr>
<tr>
<td>SR3-1</td>
<td>1.057</td>
<td>0.4</td>
<td>1.067</td>
<td>0.386</td>
</tr>
<tr>
<td>SR3-2</td>
<td>1.054</td>
<td>0.4</td>
<td>1.067</td>
<td>0.386</td>
</tr>
<tr>
<td>SR4-1</td>
<td>0.887</td>
<td>0.6</td>
<td>0.892</td>
<td>0.593</td>
</tr>
<tr>
<td>SR4-2</td>
<td>0.887</td>
<td>0.6</td>
<td>0.894</td>
<td>0.591</td>
</tr>
<tr>
<td>SR5-1</td>
<td>0.746</td>
<td>0.8</td>
<td>0.764</td>
<td>0.772</td>
</tr>
<tr>
<td>SR5-2</td>
<td>0.742</td>
<td>0.8</td>
<td>0.736</td>
<td>0.815</td>
</tr>
<tr>
<td>SR6-1</td>
<td>0.625</td>
<td>1.0</td>
<td>0.631</td>
<td>0.993</td>
</tr>
<tr>
<td>SR6-2</td>
<td>0.627</td>
<td>1.0</td>
<td>0.625</td>
<td>1.004</td>
</tr>
</tbody>
</table>

1 Sample designation
2 Theoretical thickness
3 Total theoretical effective strain
4 Measured thickness
5 Total experimental effective strain
6.3.4 Marciniak tests and strain measurement

The quasi-static forming limits of the DP600 sheet were determined using flat-punch Marciniak tests \cite{17,73} for three strain paths: uniaxial tension (UT), plane strain (PS), and biaxial tension (BT), as shown in Fig. 6.4. It has been shown that tooling, specimen geometry and the test method have minor effects on determining limiting strains \cite{74}, however, using Marciniak tests rather than Nakazima tests can eliminate some potential sources of uncertainty due to the friction between the punch and the sheet, bending and non-linear strain paths. A schematic of the Marciniak test is shown in Fig. 6.3 in which the vertical movement of the punch through a clamped sheet specimen results in in-plane biaxial deformation. In order to prevent the test specimen and the carrier blank from drawing in, a lock-bead was built into the die. Marciniak tests were conducted with a clamping force of 310 kN. The velocity of the 102 mm-diameter flat punch was set to 0.1 mm/s. To generate a uniform in-plane strain distribution on the test specimen, IF steel carrier blanks with a central hole were used. In addition, a Teflon membrane was used between the punch and the carrier blank to diminish the friction between them and ensure that the failure commences in the flat central region of the sheet metal test piece below the hole in the carrier blank. To obtain the forming limit curve (FLC) of DP600 sheet, conventional grid marking and measurement techniques were employed. After running the tests, an
optical grid analyser (model 100U from Forming Measurement Tools Innovations) was used to measure the major and minor strains. To construct the FLC, each measured grid was identified as either safe, marginal or necked on all tested UT, PS and BT specimens using the visual observation approach described by Green and Black [75] and the Keeler tactile method to detect incipient necks. Cheng [76] and Maris et al. [26] presented a detailed description of the testing procedures, specimens, tools and apparatus, measurement procedures and the experimental FLC of DP600 sheets.

### 6.3.5 Finite element model

To simulate the Marciniak tests, all tools as well as the deformable sheets were modelled precisely based on actual testing conditions and tooling dimensions. It should be noted that since the investigated DP600 does not exhibit significant anisotropic behaviour [77], the material was considered to be isotropic and due to the symmetric nature of the deformation in this test, only a quarter of the deformable bodies were modelled to reduce the computational cost. The Rousselier model including the hardening functions, void nucleation function, void coalescence criterion and void growth acceleration function was implemented in a user material subroutine (VUMAT)
Figure 6.4: Specimen and carrier blank geometries used for the experimental and FE simulations of Marciniak tests in (a) uniaxial tension, (b) plane strain and (c) biaxial tension
utilizing the Rousselier integration procedure proposed by Shterenlikht [78]. The VUMAT developed in FORTRAN95 was then used in the ABAQUS/Explicit finite element simulation software.

All the tools in the finite element model were considered to be rigid whereas the DP600 sheet test specimen and the IF-steel carrier blank were modelled as deformable bodies. They were meshed using 8-node reduced integration-brick elements (C3D8R). Symmetric boundary conditions were applied to both symmetry planes of the double-blank specimen such that the nodal displacement in the x- and z-direction were locked for the nodes located on the x- and z-symmetry planes, respectively. The geometry of different test specimens and carrier blanks used for simulating UT, PS and BT strain paths is shown in Fig. 6.4. The Coulomb friction law was determined to model the contact between surfaces using the penalty friction formulation. The coefficient of friction between the punch and the top surface of the carrier blank was set to 0.05 and that between the DP600 sheet and the IF-steel carrier blank was 0.5 [26, 79, 80]. Since no lubrication was used between the carrier blank and the blank-holder, and between the test piece and the bottom die, the friction coefficient between these surfaces was also chosen to be 0.5 and no boundary condition was considered for the outer edge of the deformable parts. A reference point was assigned to each rigid body and the boundary conditions were applied to these points, i.e. all degrees of freedom except in the velocity direction were constrained for the reference points assigned to the punch and to the blank-holder, and all degrees of freedom were locked for the bottom die. The full clamping force was directly applied to the blank-holder at the beginning of the simulation. The finite element model used to simulate the Marciniak test is presented in Fig. 6.5.
6.4 Results and discussion

6.4.1 Extended uniaxial tension flow curve

It is important to accurately describe the flow curve of materials when simulating metal forming processes since the hardening behaviour and the hardening rate need to be correctly predicted at high strain levels \[81,82\]. Therefore, uniaxial tensile tests combined with incremental rolling were used to obtain the hardening response of DP600 sheet up to a strain of 1 mm/mm. The uniaxial tension data resulting from the proposed procedure is shown in Fig. 6.6. Since most researchers utilize the hydrostatic bulge test to obtain the flow curve beyond strains that are achieved in a conventional uniaxial tension test, the true stress-true strain flow curves of DP600 obtained by hydrostatic bulge tests presented by Sigvant et al. \[65\], Uthaisangsuk et al. \[83\], Nasser et al. \[66\] and Ramazaniet al. \[3\] are also shown in Fig. 6.6 in order to examine the validity of the new test results up to high strain values. As it
can be seen, no considerable variation of flow stresses can be observed in the range of uniaxial tension test ($\varepsilon_p < 0.14$). Even beyond the ultimate tensile limit up to strain 0.7, there is very good agreement between bulge test flow curves and that achieved by uniaxial tensile tests combined with incremental rolling. Thus, it can be claimed that the proposed testing procedure is able to successfully determine the tensile flow curve of DP600 up to high strain levels and can be confidently used as the hardening behaviour of DP600 sheet in the simulations.

Figure 6.6: Comparison of the uniaxial tensile test and extended uniaxial flow curve of DP600 with the flow curve obtained by bulge tests by different researchers

Non-linear regression (NLR) was utilized to calculate the constants in the phenomenological hardening models used to simulate the Marciniak tests. It is generally known that saturated and unbounded hardening models predict the flow behaviour of materials at high strain levels differently. In addition, the total plastic strain a material can reach in strain paths other than uniaxial tension can vary significantly. Therefore, it is important to employ different hardening functions to evaluate their effect on the prediction of the FLC. In this regard, the 3-parameter Voce function, in which the work hardening becomes zero, was fitted to the uniaxial tension true-stress true-strain flow curve, and the 4-parameter Voce equation, in which stage-IV hardening is taken into account, and Ludwik’s hardening law were calibrated using the extended uniaxial
tension hardening curve. The parameters of each hardening equation, achieved by NLR, are shown in Table 6.5 and applied to the present model for DP600.

Table 6.5: Hardening parameters calculated by NLR for DP600 sheet

<table>
<thead>
<tr>
<th></th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voce (3-parameter)</td>
<td>357.90</td>
<td>748.46</td>
<td>15.035</td>
<td>–</td>
</tr>
<tr>
<td>Voce (4-parameter)</td>
<td>369.13</td>
<td>712.49</td>
<td>13.971</td>
<td>331.84</td>
</tr>
<tr>
<td>Ludwick</td>
<td>151.41</td>
<td>885.79</td>
<td>0.2517</td>
<td>–</td>
</tr>
</tbody>
</table>

To evaluate the accuracy of each hardening model to predict the flow curve of DP600 sheet, adjusted R-squared value ($\bar{R}^2$), as defined in Eq. 6.7a, was used since it can take the number of points ($m$) and the number of independent variables ($k$) into account. As it can be seen in Fig. 6.7, all three hardening models are able to accurately predict the hardening behaviour of DP600 sheet since $\bar{R}^2 > 0.97$ for the 4-parameter Voce and Ludwik’s models and close to 0.99 for the 3-parameter Voce equation.

$$\bar{R}^2 = R^2 - (1 - R^2) \frac{m}{m - k - 1}$$  \hfill (6.7a)

$$R^2 = 1 - \frac{\sum_{i=1}^{m} (\sigma_i - H(\varepsilon_p))^2}{\sum_{i=1}^{m} (\sigma_i - \bar{\sigma})^2}$$  \hfill (6.7b)

Figure 6.7: Goodness of fit of different hardening laws to the experimental flow curve of DP600 steel, evaluated by the adjusted R-squared value
6.4.2 Quasi-static formability of DP600 sheet

Several DP600 sheet specimens were deformed under uniaxial tension (UT), plane strain (PS) and biaxial tension (BT) using the Marciniak testing procedure. Grid analysis as well as visual and tactile methods were employed to determine the onset of necking such that the strain in a grid was considered safe when no necking was detected and failed when a neck could be found. Then, the analysis results were used to generate the FLC of the material as the lower bound of all necked data. In the positive minor strain region of the FLC, where obtaining a local neck is difficult experimentally, the strain on a grid immediately next to a small split was used to determine the limiting strains for such strain paths. The experimental FLC of DP600 steel sheet and the UT, PS and BT strain paths are shown in Fig. 6.8 [10]. It can be seen that the FLC\(_0\) obtained in the plane strain test was approximately 17%.

![Figure 6.8: Quasi-static forming limit diagram of DP600 steel sheet (triangles show the necked or close to split data points) [10]](image)
6.4.3 Analysis of damage evolution

The Rousselier damage model predicts the damage evolution with regard to its scalar damage variable ($\beta$) and the void volume fraction ($f$). These damage parameters will be carefully assessed in this section based on different strain paths (UT, PS and BT), various hardening functions and different void nucleation functions. It should be noted that Figs. 6.9-6.12 were derived from the output variables of an element located in the centre of the test piece. The evolution of $\beta$ as a function of equivalent plastic strain based on different testing conditions during the forming process is shown in Fig. 6.9. It can be seen that no damage was predicted if no initial void volume fraction was introduced to the Rousselier damage model (dotted lines), unlike the GTN model which is capable of predicting damage in the absence of $f_0$. However, using different void nucleation functions can significantly alter the behaviour of the cumulative damage predicted during the deformation. As shown in Fig. 6.9(a,b), the damage rate was increased by using strain-controlled void nucleation in all strain paths. In addition, for a given void nucleation function, the damage evolution in PS was predicted to be the fastest while it is the slowest in BT. Besides, all damage evolution curves which use the same void nucleation function coincided with each other up to $\varepsilon_p \simeq 0.25$ and then deviated beyond this point up to failure. Moreover, by comparing Fig. 6.9(a) and (b), it can be realized that the damage growth rate is slightly faster when using a 4-parameter Voce hardening function with cluster nucleation instead of a 3-parameter function. It should be noted that the damage evolution behaviour was reasonably similar when using either Ludwik’s or the 4-parameter Voce hardening equation. Therefore, results of only one of these functions are presented in Figs. 6.9-6.10.

Another approach that can effectively be used to assess the damage evolution predicted by the Rousselier damage model, is to evaluate the history of void volume fraction throughout the forming process. In this regard, the evolution of void volume fraction ($f$) as a function of equivalent plastic strain is shown in Fig. 6.10. Again, it can be seen that no void volume growth was predicted by the Rousselier model when using $f_0=0$. Moreover, the void growth is negligible from the beginning of the deformation up to approximately $\varepsilon_p \leq 0.2$ and $\varepsilon_p \leq 0.5$ when using cluster void nucleation and
Figure 6.9: Variation of the Rousselier scalar damage variable ($\beta$) for three strain paths (UT, PS, BT) considering 3 void nucleation cases: dotted lines (no initial void volume fracture), solid lines (cluster void nucleation) and dashed lines (strain-controlled void nucleation) using (a) 4-parameter and (b) 3-parameter Voce hardening functions.
strain-controlled void nucleation, respectively. Also, a considerable difference can be observed between the onset of sudden increase in the void volume fraction between PS and BT strain paths when using cluster void nucleation. However, this difference can be significantly reduced by using the strained controlled void nucleation function. Furthermore, the order in which the void volume growth rate increases from one strain path to another in Fig. 6.10 is similar to what was seen in Fig. 6.9 where BT and PS demonstrate the lowest and highest void volume growth rates, respectively.

These results can be explained based on the excellent experimental investigations of Tasan et al. [84] or Samei et al. [10] who performed a comprehensive study on the ductile damage mechanics and microstructural analysis of DP600 sheet deformed along different strain paths. It has been shown that a mode of PS is required to start a neck, however, in UT and BT, different constraints help to postpone the neck formation [18, 84]. Tasan et al. [84] argued that the negative minor strain in the UT and geometrical constraints in the BT can successfully help the thinning of materials, restrain the strain path inside the neck from reaching PS and delay the localization process. In addition, it has been stated that the geometrical constraints in BT are more effective at inhibiting localization than the lower triaxiality in UT. Accordingly, it can be said that the simulation results of Marciniak tests are in very good agreement with the results experimentally obtained by Tasan [84] where the rate of damage growth as a function of $\varepsilon_p$ is the highest in PS, and decreases in UT and BT due to negative minor strains and geometrical constraints, respectively.

The effect of the hardening functions on the evolution of void volume fraction in different strain paths is shown in Fig. 6.11. It can be seen that from the beginning of the deformation up to a high strain level, ($\approx 1, 0.8, 1.2$ for UT, PS and BT, respectively), all hardening models predict the same general evolution of damage when using cluster void nucleation. However, subsequent to the mentioned high strain levels, there is a remarkable difference between the evolution of $f$ predicted by the Rousselier damage model with the 3-parameter Voce law on one hand, and with the Ludwik or 4-parameter Voce hardening law on the other hand. It seems that the model employing the 3-parameter Voce hardening equation underestimates the void volume fraction, especially at high strain levels. This can be attributed to
Figure 6.10: Variation of the void volume fraction ($f$) vs. equivalent plastic strain for three strain paths considering 3 void nucleation cases using (a) 4-parameter Voce and (b) 3-parameter Voce hardening functions.
the hardening behaviour of the 3-parameter Voce function at high strain where the stress reaches a saturated level and the hardening rate becomes nil. Therefore, the model predicts a greater amount of deformation when the hardening saturates. By using the strain-controlled void nucleation function in the Rousselier damage model, these considerable differences between unbounded and saturated hardening models were significantly reduced such that the differences can be observed among different hardening models in UT (Fig. 6.11a), and PS (Fig. 6.11b), and even in BT (Fig. 6.11c), are practically insignificant.

Figure 6.11: Comparison of the void volume evolution in (a) UT, (b) PS and (c) BT vs. equivalent plastic strain for different hardening constitutive equations when using cluster void nucleation \( f_0 = \text{cte} \) and strain-controlled void nucleation \( df_N = Ad\varepsilon_p \)
6.4.4 Void coalescence criterion

The performance of a coalescence criterion can be assessed using the plastic limit load proposed by Thomason and the evolution of normalized local and homogeneous strength ($\sigma_l/\sigma_{eq}$) as a function of equivalent plastic strain, as shown in Fig. 6.12. It can be seen in this figure that the local strength between two voids decreases in all strain paths (UT, PS and BT) as the deformation progresses which indicates that it is harder for the localized mode of deformation to occur compared to the homogeneous mode. It can also be observed that the critical strain ($\varepsilon_c$) at which coalescence commences, is over-predicted by the cluster nucleation function where no secondary nucleated voids are taken into account, but $\varepsilon_c$ significantly decreased when employing strain-controlled void nucleation. This means that without considering secondary void nucleation, an element would undergo considerable deformation even after necking occurs. This is not realistic for DP600 because no significant thinning is observed after the onset of localization. In addition, regardless of the hardening function used in the model, $\varepsilon_{cPS} < \varepsilon_{cUT} < \varepsilon_{cBT}$, which can again be explained by the effect of the negative minor strain in the UT and the geometrical constraints in BT as indicated by Tasan et al. 84.

Another important point is the difference between the $\varepsilon_c$ values predicted by different types of hardening functions as they are implemented in the Rousselier model with cluster void nucleation. It can be seen in Fig. 6.12(a,b) that there is a negligible difference between $\varepsilon_c$ predicted for a given strain path using the Ludwik and 4-parameter Voce functions($\varepsilon_c \approx 0.9, 1.15$ and $1.75$ for PS, UT and BT, respectively); this indicates that the linearity or non-linearity of the hardening curve at high strain levels does not have a significant effect on $\varepsilon_c$. However, the critical strain at the onset of coalescence predicted by the 3-parameter Voce equation is significantly greater ($\varepsilon_c \approx 1, 1.25$ and $2.3$ for PS, UT and BT, respectively) than that predicted by the other hardening models under the same simulation conditions (Fig. 6.12c). Nevertheless, when using strain-controlled void nucleation, all hardening models predict approximately the same $\varepsilon_c$ for each respective strain path.
Figure 6.12: Variation of the plastic limit-load in the centre of the gauge area of Marciniak test specimens for different strain paths (UT, PS and BT) and void nucleation functions (cluster nucleation and strain-controlled nucleation) using (a) Ludwick, (b) 4-parameter Voce and (c) 3-parameter Voce hardening functions in the Rousselier damage model.
6.4.5 Strain evolution and necking criterion

The effect of the void nucleation function on the performance of the Rousselier damage model in predicting the evolution of strain during deformation can be evaluated by deriving the major strain as a function of the normalized time, as shown in Fig. 6.13. It should be mentioned that the first two terms in Eq. 6.1b basically represent the von Mises yield criterion in the Rousselier damage model. Thus, without introducing an initial void volume fraction, the Rousselier model would practically correspond to the von Mises yield criterion. It can be seen in Fig. 6.13 that in all cases, the major strain increased gradually from the beginning of deformation up to the moment \( t_{\text{norm.}} \approx 0.5 \) when the strain rate \( (d\varepsilon_I/dt) \) began to increase. Before \( t_{\text{norm.}} \), \( \varepsilon_I \) predicted by the Rousselier damage model combined with either cluster void nucleation or strain-controlled void nucleation, was the same as that predicted by the von Mises yield criterion. For both hardening models, the major strain at the location where the failure occurred, increased rapidly through the rest of the deformation when using strain-controlled void nucleation. In case of cluster void nucleation, the major strain increased similarly to that which would be predicted by the von Mises criterion, however, \( \varepsilon_I \) grew faster when using the 4-parameter Voce (Fig. 6.13a) compared with the 3-parameter Voce hardening model (Fig. 6.13b). This can again be attributed to the saturated stress condition and zero hardening rate exhibited by the 3-parameter Voce at high strain levels which contributes to greater strains at the onset of failure. The same pattern and behaviour could be observed for other strain paths and hardening functions.

Since FLC is established based on the necking strains measured in experimentally tested specimens, it is necessary to consider an appropriate and accurate approach to determine the onset of instability during the simulations that can be conveniently applied to different strain paths. In this study, a combination of different well-known necking criteria employed by different researchers to evaluate the occurrence of necking was implemented to determine FLCs [19, 79, 85]. It is generally accepted that the onset of plastic instability in a sheet metal happens when a sudden change in the thickness strain can be detected. This can be determined by deriving the first and second
Figure 6.13: Variation of the major strain during the plane strain Marciniak test using the Rousselier damage model and different void nucleation cases with the (a) 4-parameter Voce and (b) 3-parameter Voce hardening functions.

derivatives of the thickness strain based on time to obtain the acceleration of thickness deformation ($\ddot{\epsilon}_t = d^2\epsilon_t/dt^2$), as shown in Fig. 6.14(top). Since in the explicit finite element simulation, a smooth curve cannot be obtained for the $\ddot{\epsilon}_t$ versus normalized time, the second derivative of the thickness strain was first calculated by the finite difference method, and then an exponential function ($\ddot{\epsilon}_t = a \exp(bt)$) was fitted to the thickness acceleration data. Zhang et al. [79] defined the onset of plastic instability as “the intersection point of two bifurcation branches”. Therefore, a polynomial function was fitted to each branch of the fitted exponential function, i.e. the acceleration of thickness strain curve. The two fitted polynomial functions, $a_1(t)$ and $a_2(t)$ are presented in Fig. 6.14(top). The time corresponding to the intersection of $a_1(t)$ and $a_2(t)$ was considered as the critical time at which necking began. Consequently, the major and minor strains at that time were determined by spline interpolation of the closest strain values obtained from the simulations (Fig. 6.14(bottom)). The described procedure for uniaxial tension (UT) test using the Rousselier damage model, cluster nucleation and 4-parameter Voce hardening law is presented in Fig. 6.14. The same procedure was used for other strain paths, hardening equations and void nucleation functions to obtain the respective limiting strains and generate the FLC in each case.
Figure 6.14: Determining the bifurcation point from the second derivative of the thickness strain in UT using the Rousselier damage model and 4-parameter Voce hardening model, and finding the corresponding major and minor strains.

The simulation of the Marciniak tests and the subsequent bifurcation analysis to determine the necking strains in UT, PS and BT leads to the FLC shown in Fig. 6.15. As it can be seen, the FLC predicted by using the von Mises yield criterion, i.e. the Rousselier damage model with $f_0=0$, was considerably higher than either the experimental FLC or that predicted using the Ludwik, 4-parameter Voce or 3-parameter Voce hardening laws. By employing cluster nucleation, both major and minor strains decreased somewhat and the predicted FLCs moved closer to the experimental curve. When using strain-controlled void nucleation, very good agreement is observed between the predicted and experimental FLCs, such that the predicted FLC$_0$ were very close.
to the experimental value for all hardening functions. The result of predicted FLCs using the Ludwik and 4-parameter Voce hardening laws are very similar to each other. Accordingly, it can be said that the way the hardening model predicts the slope of the hardening curve at high strains has a negligible effect on the prediction of the forming limit in different strain paths. However, the results should be carefully evaluated if a saturation hardening model, such as the 3-parameter Voce, is being used. It is also worth noting that although all hardening functions could successfully predict the major and minor strains in the negative and zero minor strain region of the FLCs using strain-controlled void nucleation function, they all underestimate the necking strains in BT. Ramazani et al. [3] also reported the same deviation between the experimental and predicted FLCs on the positive minor strain side using the GTN damage model. This deviation can be attributed to the overestimation of the damage in BT or in case of Rousselier damage model, the non-transferability of the Rousselier model parameters ($D$ and $\sigma_k$) from one stress triaxiality to another [36]. However, the calibration procedure described by Sarraf et al. [61] is able to determine a single set of $D$ and $\sigma_k$ that can be used in simulations of different strain paths to obtain acceptable FLC results.

6.4.6 Necking and failure

The distribution of the cumulated scalar damage variable predicted in the Marciniak test specimens and the corresponding geometry of the neck for different simulation conditions and different strain paths is shown in Fig. 6.16. These results were also compared to the experiments. It can be seen that the location and geometry of the neck is successfully predicted by different combinations of the Rousselier damage model, hardening laws and void nucleation functions for all three investigated strain paths. In case of the Marciniak test simulating UT, all models demonstrated diffuse necking in the gauge area and strain localization in the centre of the shear bands (Fig. 6.16a). Additionally, the shape of the neck is predicted to be a line in PS (Fig. 6.16b). In the BT test specimen (Fig. 6.16c), the neck appears to start at the centre of the gauge.
Figure 6.15: Comparison of the experimental and numerically predicted DP600 FLC using the Rousselier damage model along with different void nucleation functions, and (a) Ludwick’s (b) 4-parameter Voce and (c) 3-parameter Voce hardening equations.
The predicted strain localization is more severe when the 3-parameter Voce law is used in the simulations since the stress saturates and the strain hardening rate becomes zero. Therefore, the localization of deformation and the resulting damage variable predicted by the 3-parameter Voce in all strain paths, is more severe compared to the localization predicted when employing an unbounded hardening model which can resist the softening due to the increase in void volume fraction in micromechanical damage models. Accordingly, the intensity of deformation or damage localization strongly depends on the way a hardening model predicts the strain hardening rate at high strains. Another important point is that the maximum damage level in the centre of the localized area is significantly higher when using strain-controlled void nucleation function ($\beta \simeq 5.521$ in UT and $\beta \simeq 5.973$ in PS) compared to that when cluster nucleation is utilized ($\beta \simeq 1.537$ and $\beta \simeq 2.553$ for UT and PS, respectively). This signifies that cluster void nucleation leads to an unrealistic amount of plastic deformation prior to failure (compare $\beta \simeq 1.537$ in UT at the time of the neck and $\beta_F \simeq 7.5$ at failure). The performance of the model can be noticeably improved by employing the strain-controlled void nucleation function which can increase the damage level in the localized area before the onset of coalescence and subsequent final failure. Tasan et al. [84] argued that in BT, a DP600 test specimen would experience high damage accumulation prior to necking such that the amount of plastic strain from the onset of localization to final failure would become very limited. This confirms the positive impact of utilizing strain-controlled void nucleation in the Rousselier damage model for predicting the damage accumulation in BT, as shown in Fig. 6.16c.
Figure 6.16: Representation of the Rousselier scalar damage variable ($\beta$) at the onset of necking predicted by the proposed procedure in (a) UT, (b) PS and (c) BT deformation paths using the Rousselier damage model along with different hardening models and different void nucleation functions.

The distribution of the damage in Marciniak test specimens deformed along three strain paths is presented in Fig. 6.17. It can be observed that the localization and failure commence from the centre of the specimens for each strain path, as expected from the experiments, and accordingly, fully damaged elements are removed from the simulations. However, in UT, the geometry of the final damaged specimen as well as the ultimate distribution of the damage accumulation appear to be dependent on the
hardening law, void nucleation and coalescence models that are used. When using the cluster void nucleation function and the Ludwik or the 4-parameter Voce hardening law with the Rousselier damage model, the final geometry of the damaged area was predicted to localize on the shear bands (as shown in Fig. 6.16a) but the dominant mechanism would be diffuse necking with the failure propagating from the centre to the edge of the specimen, perpendicular to the major strain direction. On the other hand, using the 3-parameter Voce hardening model would cause the UT test specimen to exhibit severe localized necking and failure on shear bands, which is similar to what was observed in the experiments (Fig. 6.17a). Nonetheless, the geometry of the damage became similar (fracture on shear bands) when the strain-controlled void nucleation function and the void coalescence criterion were employed in the model. It is worth noting that when modelling the full geometry instead of the quarter-symmetry for UT test samples, as explained in Section 6.3.5, the localization would similarly progress on the shear bands in an X-shape and the final fracture would take place on either of the shear bands.

Figure 6.17(b,c) shows the predicted geometries of the damage in PS and BT. It can be seen that all models successfully predicted the onset of necking at the centre of the specimen and its propagation outward in a direction that is perpendicular to the major strain direction. Due to the geometry of the testing sheets, no significant difference was observed between the fracture geometries predicted by the Rousselier damage model with various hardening models. However, more uniform and realistic distributions of predicted damage accumulation could be observed when utilizing strain-controlled void nucleation function in the Rousselier damage model. Nevertheless, the damage accumulation is more localized in the gauge area when using the 3-parameter Voce compared to the Ludwik and 4-parameter Voce models.
Figure 6.17: Experimental and predicted damage accumulation and distribution in (a) UT, (b) PS and (c) BT using different hardening functions and void nucleation functions (SCVN: strain-controlled void nucleation) as well as a void coalescence criterion.
6.5 Summary and conclusions

In this chapter, the performance of the Rousselier ductile damage model in predicting the formability of DP600 sheet was investigated by comparing the numerical results with experimental data. In the damage model, the work hardening behaviour of the material was defined by two approaches: uniaxial tension, and a combination of incremental rolling followed by uniaxial tensile tests to obtain the flow curve of DP600 sheet at high strain levels. Consequently, two different types of hardening laws, saturated and unbounded, were fitted to the true stress-true strain flow curves. In addition, different void nucleation functions and a void coalescence criterion were implemented in the Rousselier damage model. This model was subsequently used to simulate the Marciniak tests for three different strain paths (UT, PS and BT) to evaluate the influence of each simulation condition and each combination of functions and criteria on the predicted FLC of DP600 sheet.

Based on the comparison between the hardening curve obtained by the proposed approach of uniaxial tensile tests combined with incremental rolling with those achieved by hydrostatic bulge test, it can be concluded that this approach is an effective way of obtaining the flow curve up to high strains.

The damage evolution predicted by the Rousselier damage model, in terms of either the scalar damage variable or the void volume fraction, is remarkably strain-path dependent. It is also shown that it is also dependent on the hardening model such that the approach in which the hardening rate is predicted by a hardening model at high strain levels can directly impact the damage evolution and can lead to a considerable difference from a certain strain up to failure if cluster void nucleation function is used. However, this variability can be significantly reduced by employing the strain-controlled void nucleation function in the Rousselier damage model. It is worth noting that when using unbounded hardening models, the linearity (4-parameter Voce) or the non-linearity (Ludwik) of the hardening rate at high strain levels did not have any considerable effect on the prediction of damage increase during the deformation or damage accumulation along the gauge area.
The plastic limit load as the void coalescence criterion was successfully implemented in the model to identify the critical strain ($\varepsilon_c$) and void volume fraction ($f_c$) at the onset of coalescence. It was shown that $\varepsilon_c$ is overestimated in every strain path if the nucleation of secondary voids is not taken into account. However, using such a function can improve the performance of the coalescence criterion.

Having used the bifurcation method to determine principal strains at the onset of the necking for each strain path, the FLC of the investigated DP600 sheet was generated for each simulation condition and compared to the experimental FLC. The results showed that employing strain-controlled void nucleation function with an accurate hardening model in the Rousselier damage model allows to successfully predict the FLC of DP600 sheet with very good agreement with the experimental FLC.

Although in all simulation conditions, the onset of localization was correctly predicted to start from the centre of the gauge area, the type of hardening function and void nucleation function as well as void coalescence criterion have considerable effect on the distribution of the cumulated damage variable throughout the test specimens and on the final geometry of the fracture. Using a saturation hardening model (such as 3-parameter Voce) results in more localization around the necking area compared to unbounded models (such as 4-parameter Voce and Ludwik). In addition, utilizing a strain-controlled void nucleation function contributes to an increase in the damage distribution in the localized area as well as a decrease in the post-uniform deformation. Furthermore, the combination of the 3-parameter Voce and the Rousselier damage model predicts the final fracture on the shear bands in UT either using cluster or strain-controlled void nucleation. Finally, the final geometry of the fracture using the 4-parameter Voce or the Ludwik hardening law in the damage model was successfully improved by taking the secondary void nucleation into account in the simulations.
6.6 Acknowledgements

The authors gratefully acknowledge the financial support from NSERC-Automotive Partnership Canada (APCPJ 418056-11) program and the in-kind support from ArcelorMittal Dofasco, Natural Resources Canada, Ford Research & Advanced Engineering, Novelis Inc. and Amino N.A. Corp. Also, helpful discussions and support received from Dr. Kevin P. Boyle were much appreciated.

6.7 Bibliography


Hybrid FE+CA results and discussion

As described in Chapter 3, the proposed hybrid model is a combination of a) a finite element (FE) model that represents the macroscopic strain and stress and allows the evolving states of damage variables to be analysed in a deforming body, and b) a cellular automata (CA) model that describes the material microstructural properties and evaluates the ductile and brittle damage propagation in the meso-scale medium. In this chapter, the capabilities of the proposed model to predict the damage behaviour in terms of the fraction of ductile and brittle fracture in uniaxial tension tests and in an electrohydraulic forming process are discussed.

7.1 Microstructural properties

For each cell in the ductile CA array, the critical scalar damage variable based on the initial void volume fraction, obtained by X-Ray tomography analysis, was determined as the only cell property. However, two other properties, representing the fracture stress as a function of i) grain size and ii) grain orientation, were also defined for each cell in the brittle CA array. These properties are assigned to each cell in the CA arrays by using sophisticated random number generators based on four different
distribution functions that are available to the user:

- **uniform distribution function**: the “continuous uniform distribution” or “rectangular distribution” is a family of symmetric distributions that has constant probability. The probability density function of uniform distribution is written as:

\[
f(x) = \begin{cases} 
\frac{1}{b-a} & \text{for } a \leq x \leq b \\
0 & \text{for } x < a \lor x > b 
\end{cases} \quad (7.1)
\]

In terms of mean value of distribution ($\mu$) and standard deviation ($\sigma$), it can be re-written as:

\[
f(x) = \begin{cases} 
\frac{1}{2\sqrt{3}\sigma} & \text{for } -\sigma\sqrt{3} \leq x - \mu \leq -\sigma\sqrt{3} \\
0 & \text{Otherwise} 
\end{cases} \quad (7.2)
\]

- **normal distribution function**: the Gaussian distribution is one of the most widely-used continuous probability distributions which is usually identified with its bell-shape curve. The general equation for the probability density function of the normal distribution is

\[
f(x) = \frac{e^{-(x-\mu)/(2\sigma^2)}}{\sigma\sqrt{2\pi}} \quad (7.3)
\]

where $\mu$ is the location parameter and $\sigma$ represents the scale parameter.

- **2-parameter and 3-parameter Weibull distribution functions**: these Weibull distribution functions are other very well-known distribution functions in the engineering field. The probability density function of 2-parameter Weibull random variables is given by

\[
f(x) = \frac{\beta}{\eta} \left( \frac{t}{\eta} \right)^{\beta-1} e^{-(t/\eta)^\beta} \quad (7.4)
\]
and the 3-parameter Weibull probability distribution function is written as

\[ f(x) = \frac{\beta}{\eta} \left( \frac{t - \gamma}{\eta} \right)^{\beta-1} e^{-\left(\frac{t - \gamma}{\eta}\right)^{\beta}} \] (7.5)

where \( \eta \) is the scale parameter, \( \beta \) is the shape parameter (or slope), and \( \gamma \) denotes the location parameter.

McCallum [1] used two different techniques to determine the mean grain size of the same as-received DP600 steel sheets (i.e. taken from the same coil): the manual statistical method using Clemex Measure Line tool, and the planimetric, or Jeffries’ method. He measured more than 3000 grains to obtain the grain size distribution. Amirmaleki et al. [2] also employed Clemex Vision PE software for quantitative analysis of micrographs and ferrite grain size in the same DP600 sheets. The 3-parameter Weibull function with \( \eta=1.16 \), \( \beta=d_g=3.8 \mu m \), and \( \gamma=1.1 \) was fitted to the experimental data and employed in the model to determine the fracture stress, as shown in Fig. 7.1.
Figure 7.1: (a) grain size measurements using Clemex [1] and (b) distribution of ferrite grain size in DP600 sheet specimens.

The distribution of initial void volume fraction was obtained by high resolution X-ray tomography of as-received DP600 steel sheet specimens. The tomography acquisition
was performed with a voxel size (the relative spacing of volume-elements) of 0.6 µm. Accordingly, a normal distribution function with a mean value of $\mu = \bar{f}_0 = 0.0006$ and a standard deviation of $\sigma = 0.00013$ was used to assign the initial void volume fraction and its corresponding critical Rousselier scalar damage variable ($\beta_f$), based on Eq. 5.1d to each cell in the ductile CA array (as shown in Fig. 7.2).

![Histogram and Normal Distribution Curve](image)

**Figure 7.2:** Overall distribution of $\beta_f$ calculated based on $f_0$

No direct measurements were carried out to determine the grain orientation in the investigated DP600 steel sheets. Since the grain orientation is employed to determine the crack arrest phenomenon, the grain orientation angle ($\alpha$) and the misorientation threshold ($\alpha_c$) reported by Bhattacharjee et al. [3, 4] and Shterenlikht et al. [5, 6] was utilized in the current model. Accordingly, a uniform distribution of grain orientations with $0^\circ \leq \alpha \leq 70^\circ$ was used to assign the grain orientation class to each cell in the brittle CA array and $\alpha_c=30^\circ$ was chosen to be the misorientation threshold in this model, i.e. the absolute value of the difference between grain orientations in two neighbouring cells in the brittle CA array should be less than this misorientation threshold to allow the brittle fracture to propagate from one cell to another, otherwise the brittle fracture (or the crack) would be arrested and cannot propagate. In addition,
the uniform distribution function was used to determine the location of Alive\(_m\) cells (martensite containing cells) and ferrite grain size.

### 7.2 Illustration of the performance of the model

In order to demonstrate the performance of the hybrid FE+CA model in a comprehensible approach, a single finite element located in the centre of an ASTM-E8M specimen, was chosen to investigate the ability of the model to predict the damage behaviour in quasi-static uniaxial tension, as shown in Fig. 7.3a. The mechanical properties of DP600 sheet specimens used in the FE part are shown in Table 7.1. The work hardening behaviour was defined using the modified Johnson-Cook model (Eq. 4.4) and the coefficients are shown in Table 7.2. Furthermore, the material constants for the Rousselier damage model were found to be \(D=2.5\) and \(\sigma_k=425\) MPa for this DP600 sheet.

#### Table 7.1: Mechanical properties of as-received DP600

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<td>(\rho)</td>
<td>(\sigma_y)</td>
<td>(\sigma_{UTS})</td>
<td>(\varepsilon_{UTS})</td>
</tr>
<tr>
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<td>((\text{kg/m}^3))</td>
<td>((\text{MPa}))</td>
<td>((\text{MPa}))</td>
<td>(\text{s}^{-1})</td>
<td></td>
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<tr>
<td>210</td>
<td>0.3</td>
<td>7800</td>
<td>340</td>
<td>587</td>
<td>0.176</td>
<td>0.001</td>
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#### Table 7.2: Coefficients of mJC hardening function for DP600

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<th>(C_4)</th>
<th>(C_5)</th>
</tr>
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<tbody>
<tr>
<td>modified JC (mJC)</td>
<td>225.35</td>
<td>850.16</td>
<td>0.3194</td>
<td>0.0037</td>
<td>1.5715</td>
</tr>
</tbody>
</table>

In view of the correlation between ductile and brittle damage cell sizes (described in Section 3.2) and the mean ferrite grain size, \(L_d\) and \(L_b\) were chosen to be 0.2mm (0.1mm < \(L_d\) < 0.5mm) and 0.05mm (\(L_b\) is usually 10-20 times larger than the median grain size), respectively. According to Eqs. 3.1 and 3.3, the size of FEs in each direction was chosen to be 0.55mm so that each ductile CA array was made up of 64 cells and
each brittle CA array consisted of 512 cells for every single FE in the gauge area. At the beginning of the simulation, random number generators are employed to assign $\beta_f$ values to each cell in the ductile cell array, and likewise for assigning values for $\sigma_f$ and $\alpha$ to each cell in brittle cell array. In addition, all cells in the ductile and brittle cell arrays are initially *Alive* since no damage or failure has occurred yet. Since there is about 5% martensite in DP600 specimens, approximately the same proportion of $Alive_m$ was assigned to the brittle cells in order to take into account the martensite during the damage evolution. It is worth noting that cells, either in the ductile or brittle CA array, are not individual phases in the microstructure. Rather, cells are sub-element size parts of the material with homogeneous yet unique material properties, i.e. microstructural properties are different in each cell but there are no individual microstructural phases present in the cells. According to meso-scale modelling concepts, cells do not represent ferrite grains or martensite islands in this model, and the boundaries of cells do not denote grain boundaries or ferrite/martensite interfaces. Consequently, no separate constitutive equations or crystal plasticity theories are needed to define the mechanical properties of ferrite and martensite as it would in a micro-mechanical model (which is hard to obtain). Instead, one constitutive model is utilized to simulate the deformation and damage behaviour of the material at the macro-scale (FE-scale) and determine macro-level strain, and microstructural properties can be used to track the damage evolution and failure mechanisms in meso-level. The 2D and 3D representation of ductile and brittle cell states are shown in Fig. 7.3(b,c) and Fig. 7.3(d,e), respectively.
As the deformation progresses, output values from the FE part of the simulation, i.e. the macro-scale scalar damage variable ($\beta$) and the maximum principal stress ($\sigma_I$) shown as a solid red line in Fig. 7.4-7.7 (top images-solid line), start to change and usually increase based on the strain path. At a certain point, the FE output (either of the solid red lines) reaches one of the critical values implemented in one of the cells.
in either the ductile or brittle CA array and consequently, changes its cell state from *Alive* to *Dead* in the case of the ductile cell array, or from *Alive* or *Alive*$_m$ to *Dead*$_b$ in the brittle cell array, according to the associated full transfer rule defined as an essential part of the CA model.

When a cell state changes from *Alive* or *Alive*$_m$ to *Dead*$_d$ or *Dead*$_b$ due to the ductile or brittle fracture criterion, some cells in the vicinity of the dead cell, i.e. those located close to the plane normal to the maximum principal stress should carry a greater share of the damage which means that these particular neighbouring cells are more vulnerable to damage propagation compared to other neighbouring cells. Accordingly, local concentration factors are defined for the ductile cell array ($C_D$) and the brittle cell array ($C_B$) to take into account the effect of dead cells on their neighbouring cells. As the equivalent plastic strain increases (from Fig. 7.4-7.5), both $\beta$ and $\sigma_I$ (represented by the solid red lines) increase until they reach $\beta^m_I$ or $\sigma^m_I$ respectively, in cell $m$ and the value of the damage variable in neighbouring cells will decrease and the corresponding blue data points will move down towards the red line because they must accommodate an increased share of damage due to the dead cell in their vicinity.

![Figure 7.4: FE input from ABAQUS solver (solid red lines in top figures) and (a) critical scalar damage variable in ductile cells and (b) fracture stress in brittle cells (blue dots) during uniform deformation in the gauge of a tensile specimen](image)
Figure 7.5: FE input from ABAQUS solver (solid red lines in top figures), and (a) critical scalar damage variable in ductile cells and (b) fracture stress in brittle cells at the onset of localization and necking.

Described procedure starts from the beginning of the simulation and continues during the deformation until the number of dead cells in either of the CA arrays reaches a predefined value. In the absence of coalescence, all brittle and ductile cells would need to become dead before the element would lose its load-carrying capacity and be removed from the simulation. However, this assumption is not realistic, therefore a coalescence criterion is implemented so that the entire array becomes dead and subsequently the element is removed from the mesh when the number of dead cells, either ductile or brittle, reaches a critical number \( X_{max}^{(d)} \) or \( X_{max}^{(b)} \), respectively) that is less than the total number of cells in the array. Based on material failing due to the presence of a planar crack, the coalescence criterion is defined as a function of the number of dead cells on a plane that is perpendicular to one of the three principal directions \( X^{max} = D^{2/3} \) [5, 6]. It can be seen in Fig. 7.7 that final failure can occur earlier when coalescence is included in the CA part of the simulation (the fracture strain reduces to \( \simeq 0.4 \) which is very close to what is measured in the experiments):
Figure 7.6: Number of dead cells required for the entire brittle CA array to be considered dead (a) without coalescence criteria and (b) with a coalescence criterion

Figure 7.7: FE input from ABAQUS solver (red lines in top figures), and (a) critical scalar damage variable in ductile cells and (b) fracture stress in brittle cells at the time of failure

The same procedure can be followed to evaluate the performance of the hybrid FE+CA model in other strain paths such as pure shear, simple shear, compression and successive tension-compression tests. As mentioned in Section 2.3.4, one of the most important advantages of the Rousselier damage model over the GTN model is its ability to predict
damage growth at very low, zero or negative stress triaxiality. It can be deduced from Fig. 7.8 that under zero stress triaxiality, the Rousselier damage variable (solid red line) increases as deformation progresses. Therefore, even the original Rousselier damage model (with or without the CA model) can predict damage evolution in either pure shear or simple shear, and generally predict final failure in a wide range of stress triaxialities when calibrated accurately.

Figure 7.8: FE input from ABAQUS solver (red lines), and critical scalar damage variable in ductile cells in (a) simple shear and (b) pure shear tests

7.3 Parametric study

In this section, the uniaxial tension test is modelled using the modified Rousselier constitutive damage model for the FE-scale part and the hybrid FE+CA model for predicting the evolution of ductile and brittle damage mechanisms. To evaluate the performance of the proposed model, a series of parametric studies was conducted to investigate the effect of martensite volume fraction, ferrite grain size, strain rate and temperature on the failure behaviour of the miniature dog-bone tensile specimens. The simulations were carried out for strain rates of 1 and 1000 s\(^{-1}\). Accordingly, DP600 and DP780 steels with nominal martensite volume fractions of 5% and 25%, respectively,
were chosen as the main materials for this study. And different ferrite grain sizes ranging from ultra fine-grained to coarse-grained were considered as the microstructural properties of the materials. The capability of the hybrid FE+CA model to predict the fraction of ductile and brittle fracture in each case is demonstrated and discussed, and related experimental evidences are compared to the predicted results. To facilitate the parametric studies, different Python and MATLAB codes as well as scripting techniques were employed to derive and post process the simulation data.

According to the conventional finite element simulation method, only a quarter of the cross section (1/8 of specimen) can be modelled to reduce the computational cost due to the symmetries associated with the material and test geometry. In this approach, the uniform and post-uniform deformation of the specimen would be symmetric and even the predicted fracture surface would not show any asymmetry since no microstructural properties or material heterogeneity is associated with the FE properties. However, in the following examples, half of the cross sectional area (or a quarter of the specimen) was modelled to see if the proposed model was capable of predicting any non-symmetry of the final fracture surface. Detailed descriptions of the size of the specimens and of the different techniques and approaches employed for finite element analysis of the uniaxial tension test using the miniature dog-bone specimens are presented in Chapter 4 and 5. The FE model of the miniature tensile specimen is shown in Fig. 7.9. It should be noted that to reduce computational cost, the hybrid FE+CA model was employed just in a specific part of the gauge area where the damage is more probable to develop, as shown in Fig. 7.9a. The 12 elements on the cross-section of the specimen that are shown above the symmetry line in Fig. 7.9b will be reproduced figures throughout this section so as to display the results predicted by the FE+CA hybrid model.
For both DP600 and DP780, the Young’s modulus, Poisson’s ratio and the density were $E=210$ GPa, $\nu=0.3$ and $\rho=7800$ kg/m$^3$, respectively. Also the appropriate Rousselier model parameters were calculated to be $D=2.5$ and $\sigma_k=425$ MPa for DP600 and $D=2.5$ and $\sigma_k=735$ MPa. The material work hardening properties were described by the Khan-Huang-Liang (KHL) hardening law, and the coefficients for the hardening functions can be found in Table 7.3.

Table 7.3: Coefficients of KHL hardening function for DP600 and DP780

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<tr>
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<th>$C_1$</th>
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<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
<th>$C_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP600</td>
<td>161.54</td>
<td>946.48</td>
<td>0.2577</td>
<td>-0.1900</td>
<td>0.0037</td>
<td>-</td>
</tr>
<tr>
<td>DP780</td>
<td>500</td>
<td>1603</td>
<td>0.4135</td>
<td>0.01</td>
<td>0.01632</td>
<td>1.514</td>
</tr>
</tbody>
</table>

In the gauge area, a $5\times5\times5$ ductile cell array ($D_d = 125$) and a $10\times10\times10$ brittle cell array ($D_b = 1000$) were assigned to each FE so that the ductile cell size was calculated to be $L_d=0.075$ mm and the brittle damage cell was considered to be $L_b=0.02$ mm. The two-parameter Weibull distribution random number generator, with a shape parameter $W_\beta=0.0007$ and a scale parameter $W_\eta=0.00025$, was employed to simulate the distribution of initial void volume fraction, and is then used to generate $\beta_f$ (as a function of initial void volume fraction as shown in Eq. 5.1d) understructural
array for ductile CA array (Fig. 7.10a). The fracture stress value in each cell in the brittle CA array was assigned by a 3-parameter Weibull random number generator with $W_\eta=1.16$, $W_\beta=d_g=3.5 \mu m$ and $W_\gamma=1.1$. Only $W_\beta$ was changed when the ferrite grain size changed and other parameters in the 3-parameter Weibull function remained constant. The same grain orientation angle and misorientation threshold as presented in Section 7.2 were used in the following examples. A 3D representation of the fracture stress and grain orientation angles are shown in Fig. 7.10(b,c).

![3D representation](image)

Figure 7.10: 3D representation of initial understructural arrays of (a) critical Rousselier scalar damage variable for ductile CA array, (b) fracture stress and (c) grain orientation for brittle CA array

The effect of grain size and strain rate on the fracture surface of DP600 sheet specimens in uniaxial tension is shown in Fig. 7.11. It should be mentioned at the onset that the
predicted percentage of brittle fracture ($\%F_b$) in the following examples is provided for qualitative comparison, and further detailed investigation is required for quantitative evaluation of ductile and brittle fracture on the fracture surface. It can be seen in Fig. 7.11 that the fraction of brittle fracture ($\%F_b$) for both fine- and coarse-grained DP600 is negligible when the test is carried out at low strain rate, although, a slight increase in $\%F_b$ can be observed when the ferrite grain size increases. The brittle fracture percentage also increases with an increase in strain rate. Nevertheless, with a martensite volume percentage as low as 4.7% in DP600 and a fine ferrite grain size, the $\%F_b$ remains very low and the dominant fracture mechanism is ductile. This is in very good agreement with the experimental results reported by Samei et al. [8, 9] and shown in Fig. 7.12. Quasi-cleavage fracture is distinct from cleavage fracture since dimples and tear ridges can be observed around the periphery of the facets [8, 10, 11]. However, the amount of brittle fracture observed in low- and high-strain rate deformation of DP600 sheet specimens is not significant compared to the percentage of ductile fracture where the dominant presence of dimples on the fracture surface indicates that ductile fracture is predominant.
Figure 7.11: Fraction of brittle fracture in (a,c) fine-grained ($d_g=3 \, \mu m$) and (b,d) coarse grained ($d_g=6.5 \, \mu m$) DP600 specimens

Figure 7.12: Quasi-cleavage (Q) fracture on the fracture surface of DP600 tested under quasi-static condition [9]
Figure 7.13 shows the fraction of brittle fracture in quasi-static and high strain rate deformation of fine- and coarse-grained DP780. The same results can be observed in this figure where an increase in either ferrite grain size or strain rate results in an increase in $\%F_b$. However, the combined result of high-strain rate deformation on the coarse-grained DP780 lead to a significant amount of brittle fracture. Therefore, the major fracture mechanism is predicted to be a combination of ductile and brittle fracture. Samei observed quasi-cleavage fracture in fine-grained DP600 subjected to quasi-static deformation and to high-strain rate electrohydraulic forming (EHF), as shown in Fig. 7.14(a,b), respectively. He also stated that the amount of cleavage fracture and the number of facets were greater in DP980 with higher martensite content, and it was observed more frequently in the EHF process which confirms the qualitative predictions of the proposed model.

![Figure 7.13](image.png)

Figure 7.13: Fraction of brittle fracture in (a,c) fine-grained ($d_g=3 \mu m$) and (b,d) coarse grained ($d_g=6.5 \mu m$) DP780 specimens
Figure 7.14: Quasi-cleavage (Q) fracture on the fracture surface of DP780 deformed (a) under quasi-static conditions and (b) at high-strain rate [8].

Figure 7.15 shows the comparison between the average percentage of brittle fracture in fine- and coarse-grained DP600 and DP780 subjected to low- and high-strain rate uniaxial tension. It can be clearly seen that an increase in either the martensite volume fraction, the ferrite grain size or the strain rate lead to an increase in the percentage of brittle fracture. Several researchers have stated that the coarse-grained dual phase structures have much lower elongation (ductility) and higher tendency to experience brittle fracture due to the initiation of cleavage cracks in the ferrite matrix [12,14]. It has also been shown that dual phase steels exhibit relatively less ductile damage failure and more brittle fracture as the volume percentage of martensite increases [8,14,15]. Therefore, the combination of higher martensite volume content with coarse-grained ferrite and high-strain rate deformation can contribute to increased brittle fracture.
Figure 7.15: Total fraction of brittle fracture predicted in fine-grained and coarse-grained DP600 and DP780 at low and high strain rates

Calcagnotto et al. \cite{16} performed a study on the mechanical properties and failure behaviour of a dual phase steel with a martensite volume percentage somehow close to the DP780 steel that is being considered in this section. They generated different thermomechanical processing routes to produce ultrafine-grained (UFG), fine-grained (FG) and coarse-grained (CG) dual phase steels with a ferrite grain size of 1.5, 3 and 12 μm, respectively. Then, tensile tests were used to evaluate the deformation and damage behaviour of each type of DP steel. Their test results showed that in UFG steel (Fig. 7.16b) the main fracture mechanism was ductile damage since void nucleation and growth processes resulted in a uniform distribution of dimples throughout the fractured area. On the other hand, FG steel exhibited ductile fracture with some cleavage planes among the ferrite grains (Fig. 7.16d). Therefore, although the main fracture mechanism was still ductile, some parts of the specimen exhibited brittle fracture. In case of CG steel, no post-uniform elongation was observed and the dominant fracture mechanism was found to be brittle with facets and cleavage steps on these facets (Fig. 7.16f). The fracture mechanisms predicted by the proposed model are in very good agreement with the experimental results obtained by Calcagnotto et al. \cite{16}. As Fig. 7.16a shows, the main fracture mode in UFG steel is predicted to be ductile with some possible quasi-cleavage facets ($F_b \approx 2.7\%$). In FG steel, the proportion of brittle fracture increased ($F_b \approx 15\%$) and the fracture surface exhibited a combination of ductile and brittle fracture (Fig. 7.16c). Lastly, $F_b$ increased significantly ($F_b \approx 75\%$) for CG steel.
and brittle fracture is found to be the dominant failure mechanism when simulating a tensile test, as shown in Fig. 7.16e.

Figure 7.16: Comparing the effect of grain size on the predicted fraction of brittle fracture and related experiments in (a,b) ultra-fine grained ($d_g=1.5 \, \mu m$), (c,d) fine-grained ($d_g=3 \, \mu m$) and (e,f) coarse-grained ($d_g=12 \, \mu m$) DP780 specimens (fracture surface images are from Calcagnotto et al.[16]).

Initial and final cell states in the brittle CA array are additional outputs of the proposed model that can be discussed. Figure 7.17 shows the initial brittle cell states and the distribution of $Alive_m$ cells in each finite element for the DP780 specimen.
is well-established that in conventional finite element modelling of uniaxial tension test, only an eighth of tensile specimens needs to be modelled due to the symmetrical configuration of the specimens and the nature of deformation in order to reduce computational cost [17]–[20]. However, the damage and fracture predicted with the hybrid FE+CA model are not symmetric since the damage mechanisms are decoupled from the FE model and transferred to ductile and brittle cell arrays with asymmetric and randomized microstructural properties. This is the main reason that neither the predicted brittle fracture percentages shown in Fig. 7.11–7.16 nor the distribution of dead cells in Fig. 7.18 are symmetric; this is no doubt more realistic.

The final cell states in the brittle CA array along with Alive$_m$ cells are shown in Fig. 7.18. Since no void shape is specified in this model, it can account for volumetric void growth but is not capable of predicting void shape changes. As can be seen in Fig. 7.18a, the main fracture mechanism in UFG-DP780 specimen is ductile since most cells in the brittle CA array are dead due to the ductile fracture criterion (yellow circles) although a very small number of Dead$_b$ cells (red circles) are present. The number of Dead$_b$ cells increased in the FG specimen showing that there is a competition between two fracture modes that will determine which one will become the dominant mechanism for failure. Another important point that can be observed is the location of Dead$_d$ and Dead$_b$ cells relative to each other (particularly in the UFG specimen) where dead cells due to the brittle fracture criterion (Dead$_b$) are surrounded by Dead$_d$ cells. These cells can be considered representations of quasi-cleavage which has been observed in DP780 sheet specimens [8]. The relatively high number of red circles (Dead$_b$ cells) in Fig. 7.18b reveals that the significant increase in the size of ferrite grains altered the main fracture mechanism from ductile to brittle.
Figure 7.17: Initial brittle cell states in each FE located on the cross-section of the DP780 miniature dog-bone specimen
Figure 7.18: Final brittle cell states in each FE located on the cross-section of (a) ultra-fine grained ($d_g=1.5 \, \mu m$) and (b) coarse-grained ($d_g=12 \, \mu m$) DP780 specimen
Other parametric studies that can be performed using the proposed model are the evaluation of the effect of temperature and mean ferrite grain size on the fraction of brittle fracture. Subsequently, sigmoid curves can be fitted to the predicted results and the effect of both transient temperature and the grain size (for a specific strain rate) on the fraction of brittle fracture can be determined. The fraction of brittle fracture as a function of temperature shown in Fig. 7.19 indicates that ductile fracture will become the dominant fracture mechanism even for a coarse-grained DP780 with mean ferrite grain size of $d_g=12$ µm, deformed at high strain rate provided that the test is carried out at temperatures greater than 80°C. Other researchers also reported the same effect on other dual phase steels [15, 21]. The predicted fracture behaviour as a function of temperature is in good agreement with the experimental results obtained by Calcagnotto et al. [16] for CG-DP780 subjected to quasi-static deformation. Also it can be seen from Fig. 7.20 that $F_b$ does not change with strain rate for DP780 with a ferrite grain size of less than 6 µm. This is the threshold grain size beyond which the combined effect of high strain rate and greater grain sizes would lead the brittle fracture mode to be the dominant failure mechanism.

![Graph showing the effect of temperature on the fraction of brittle fracture in coarse-grained (d_g=12 µm) DP780 specimen at \( \dot{\varepsilon}=1000 \, s^{-1} \)](image)

Figure 7.19: The effect of temperature on the fraction of brittle fracture in coarse-grained (d_g=12 µm) DP780 specimen at \( \dot{\varepsilon}=1000 \, s^{-1} \)
7.4 Simulation of electrohydraulic forming (EHF)

High strain rate deformation is a very effective approach to increase the formability of sheet metals beyond their conventional limits, decrease wrinkling, and reduce springback [22, 25]. It has been shown that inertial effects, and die impact effects are the main sources of formability improvement in high strain-rate forming conditions [26, 27]. Different techniques and technologies such as explosive forming (EF), electromagnetic forming (EMF), and electrohydraulic forming (EHF) can be used to deform materials under high energy rate forming (HERF) processes [23, 25, 28, 29]. The main difference between EF, EMF and EHF forming processes is the source of energy and the procedure in which the released energy deforms a sheet. In explosive forming, chemical explosives, usually immersed in water, provides the forming energy, whereas in EMF, energy stored in high-voltage capacitors is released through a multi-turn coil located near the sheet so that the sheet can be formed due to magnetic repulsive forces.
Electrohydraulic forming (EHF) is a high-energy rate forming process that directly convert electrical energy into mechanical force that can form a sheet material. In EHF, high-voltage electrical energy stored in capacitors is discharged between two electrodes that are submerged in a water-filled chamber in order to generate a high-energy shock wave in the water and force the sheet metal into the die cavity. The entire process can be completed within a few hundred microseconds depending on the positioning of the electrodes and the applied energy. Different materials exhibit different forming and damage behaviour when they are deformed in free-forming (EHFF) or die-forming (EHDF) conditions. Figure 7.21 shows a schematic of EHFF and EHDF tooling. A detailed review of the EHF process, tools and apparatus, material behaviour and measurement procedures, and simulation methods have been reported by Rohatgi et al. [25, 30–32], Gillard et al. [29], Hassannejadasl et al. [33, 34], and Maris et al. [35, 36].

Due to the significant number of fractured specimens in electrohydraulic free forming [34], only the simulation of electrohydraulic free forming (EHFF) is presented here. To simulate the EHFF process, one quarter of the die, the blank-holder and the DP600 metal sheet were modelled precisely due to the symmetry of the process based on actual testing conditions and tooling dimensions. No significant planar anisotropy was detected for DP600 sheets [37], therefore, the test specimen was considered to be isotropic. All tools in the finite element model were considered to be rigid bodies while the DP600 sheet specimen was modelled as a deformable body and was meshed
using reduced integration three-dimensional Lagrangian solid elements (C3D8R in the
ABAQUS element library). To apply symmetric boundary conditions to the symmetry
planes of the DP600 specimen, the nodal displacement in the x- and z-direction were
constrained for the nodes located on the x- and z-symmetry planes, respectively. A
reference point was assigned to each rigid body and the boundary conditions were
applied to these points, i.e. all degrees of freedom except in the velocity direction were
constrained for the reference points assigned to the blank holder, and all degrees of
freedom were locked for the die. The finite element model used for simulating EHFF
is shown in Fig. 7.22.

![Finite element model of the EHFF](image)

Figure 7.22: Finite element model of the EHFF. From top to bottom: blank holder,
sheet specimen and lower die

To simulate the EHF and model the water pressure, Golovashchenko et al. [38]
and Rohatgi et al. [32] defined the pressure profile (as shown in Fig. 7.23) as an
exponentially decaying function of time as follows:

\[ P(t) = P_0 \left( \frac{t}{\delta} \right)^a \exp \left( -\frac{bt}{\delta} \right) \]  

(7.6)
where $P$ is the time-dependent pressure, $P_0$ denotes peak pressure amplitude, and $t$ represents time. $N_p$, $\delta$, $a$ and $b$ are function constant. For the simulation of EHFF in this study, the values of $N_p=1.28$, $\delta=150$ $\mu$s, $a=0.089$, and $b=0.53$ were determined. These values were calculated based upon iterative parametric studies and by comparing the experimental strains, strain rates and dome-height to predicted ones. Rohatgi et al. [32] also postulated that the non-uniform distribution of pressure over the sheet can be determined by the following linear function:

$$P(x, t) = P(t) \left(1 - \frac{x}{2R}\right) \quad 0 \leq x \leq R$$  \hspace{1cm} (7.7)

where $R$ is the radius of the circular region over which the test sheet is subjected to the pressure-pulse. However, Gillard et al. [29] used a rigorous multi-physics model of EHF to simulate the pressure wave inside the water chamber and showed that the pressure distribution pattern, caused by the plasma channel between the electrodes, has a spherical shape at the beginning of the EHF process. In addition, Hassannejadasl et al. [34] and Maris et al. [36] modelled the water with Eulerian elements and assumed that the pressure wave that propagates through the water becomes hemispherical in shape after the electrical discharge. As it can be seen from Fig. 7.24(a,b), they accelerated a
set of nodes in the water which lie on a hemispherical surface to model the shockwave growth and propagation. Therefore, the linear function Rohatgi et al. 32 utilized to model the pressure distribution in EHF does not seem realistic. Thus, Eq. 7.7 is modified to model the pressure distribution on the sheet specimen with a non-linear non-uniform function (Eq. 7.8) to make the pressure distribution change smoothly from the centre to the edge of the sheet specimen. 2D representation of EHFF and different approaches to define the pressure-pulse distribution on the sheet specimen is shown in Fig. 7.25.

\[
P(x, t) = P(t) \left[ 1 - \left( \frac{x}{2R} \right)^2 \right] \implies 0 \leq x \leq R
\]

Figure 7.24: Nodal acceleration in the water used by (a) Hassannejadasl et al. 34 and (b) Maris et al. 36 to simulate EHF (NB both schematic figures are shown upside down)
It is worth noting that the described formulation does not account for the complexities of pressure-wave reflections in the water chamber and the test specimen. More advanced models can be found in recent publications [29, 31, 36], however, the main objective of the current study is to address the capabilities and the performance of the proposed FE+CA model in predicting the forming behaviour, and the damage and failure behaviour of sheet metal specimens subjected to EHF. Therefore, utilizing this simplified model was considered sufficient to fulfil the present purposes. Nevertheless, good agreement between experimental data obtained by Hassannejadasl et al. [34] and Maris et al. [36] and the predictions of the current proposed model was observed.

Figure 7.26 (a,b) shows the predicted strain paths at various locations relative to the apex in EHFF for two different levels of applied energy. It can be seen that the strain path close to the apex is equibiaxial, however, it deviates from equibiaxial tension as the location changes radially from the centre of the specimen to the outside edges. Nevertheless, equibiaxial strain paths can be seen in all locations at the very beginning of the deformation ($\varepsilon_I < 0.04$). Comparing Fig. 7.26a with Fig. 7.26b reveals that increasing the input energy leads to greater major strain values. These results are
in good agreement with the experimental results published by Rohatgi et al. [32] and the results predicted using an Eulerian-Lagrangian approach and published by Hassannejadasl et al. [34].

The predicted effective plastic strain rate history at different locations on the sheet in EHFF at different charging voltages is presented Fig. 7.26(c,d). It can be seen that the maximum effective strain rates were obtained at the apex of the specimen and were approximately 2700 s\(^{-1}\) and 3050 s\(^{-1}\) for 9.2kV and 10.3kV tests, respectively. It is worth noting that using higher voltage, hence greater input energy, for EHFF results in an increase in the strain rate but the overall profile of the strain rate vs. time curve remains unchanged.

Figure 7.26: (a,b) Predicted strain path and (c,d) predicted effective strain rate history in EHFF for two different levels of input energy
Figure 7.27 shows the predicted histories of the Rousselier scalar damage variable ($\beta$), the equivalent plastic strain, and the stress-triaxiality factor in an element located at the apex of the fractured DP600 sheet specimen. Despite some variation at the beginning of the simulation, the stress-triaxiality history shows an average value of 0.66 during the deformation due to the equibiaxial condition at the apex of the specimen. The equivalent plastic strain shows a smooth and continuous increase throughout the simulation. It can also be seen that $\beta$ is approximately zero at the beginning of the deformation but from $t \approx 80 \mu s$, it increases continuously up to a critical value where complete loss of load bearing capacity occurs. In conventional finite element simulations, the critical damage variable would be a function of process parameters such as stress triaxiality, therefore in similar testing conditions, this critical value would not change whatsoever. However, since the control of the damage and failure is transferred from the FEs to the cell arrays in the proposed hybrid FE+CA model, even elements subjected to similar strain path and stress triaxiality conditions, would exhibit different damage behaviour.

![Graph showing predicted histories of plastic strain, Rousselier scalar damage variable and triaxiality](image)

Figure 7.27: History of plastic strain, Rousselier scalar damage variable and triaxiality in a damaged element at the apex of DP600 sheet subjected to EHFF

Figure 7.28 shows the experimental and predicted damage accumulation and final damage geometry of fine-grained DP600 sheet specimen in a failed EHFF specimen
deformed with 13.6kJ energy input. Severe fracture and tearing starting from the apex of the specimen were observed due to the absence of a die and the high energy input released from the electrodes, as shown in Fig. 7.28a. The model predicted the damage to initiate from the apex and propagate radially toward the edge of the specimen. It can be seen that there is good agreement between the experimental and predicted geometry of damage for fine-grained DP600. Figure 7.30 shows the total percentage of brittle fracture in damaged elements in fine- and coarse-grained DP600 sheets deformed by EHFF. It can be seen that only around 6.5% of the fracture is predicted to be brittle fracture so it can be concluded that the dominant failure mode in this case was ductile fracture. A thorough fractography analysis of the fracture surfaces was carried out by Samei and revealed that ductile fracture was the dominant type of fracture in all EHFF specimens, although he observed a limited amount of quasi-cleavage fractures in DP780 sheet specimens deformed under EHFF.

The effect of increasing the input energy and the ferrite grain size on the damage accumulation and geometry of DP600 specimens subjected to EHFF can be seen in Fig. 7.29. According to Fig. 7.29a and Fig. 7.30, increasing the applied energy from 13.6kJ to 15.6kJ slightly changed the geometry of the fractured specimen but the fraction of brittle fracture still remains less than 0.1 which indicates that the major fracture mode is still ductile although the deformation rate is increased. On
the other hand, the dominant failure mechanism when using lower energy for a coarse-grained DP600 specimen, was predicted to be brittle since less than 15% of cells were predicted to be dead due to ductile fracture. In the latter case, a severe circumferential crack formed near the apex of the specimen and the damage propagated in different directions.

Figure 7.29: Predicted damage geometry of fracture in DP600 specimens (a) 10.3 kV (15.6 kJ), \( d_g = 3.5 \) µm and (b) 9.2 kV (13.6 kJ), \( d_g = 12 \) µm

Therefore, it can be seen that increasing the input energy of the EHFF process or the ferrite grain size of the DP steel sheet specimen results in a significant change in the final geometry of the fractured surface and the dominant damage mechanism from ductile to brittle mode.

Figure 7.30: Total predicted fraction of brittle fracture in fine-grained and coarse-grained DP600 subjected to EHFF with different applied energy values

Therefore, it can be seen that increasing the input energy of the EHFF process or the ferrite grain size of the DP steel sheet specimen results in a significant change in the final geometry of the fractured surface and the dominant damage mechanism from ductile to brittle mode.
7.5 Bibliography


Overall summary and conclusions

8.1 Overall summary

The current study was conducted to predict the forming behaviour and the onset of instability and failure by developing a microstructurally-based constitutive model and implementing it in a commercial finite element simulation software. Moreover, the concept of a combined finite element analysis method with cellular automata was found suitable for this purpose. Accordingly, in the first step, the Rousselier model was chosen as the main micromechanical continuous ductile damage model and was modified by including secondary void nucleation models, physical microvoid coalescence criteria and a void growth acceleration function. Using the mechanical properties obtained from uniaxial tension tests at strain rates ranging from 0.001 s\(^{-1}\) to 1000 s\(^{-1}\), a comprehensive study was then carried out to evaluate the performance of integrated or multiplicative rate-sensitive work hardening functions in predicting the hardening behaviour of dual phase steel sheets. In addition, Marciniak tests were performed on a number of DP600 sheet specimens to obtain the forming limit curve (FLC) and evaluate the forming behaviour of DP600 along different strain paths. Also, X-Ray tomography analysis was employed to evaluate the void volume fraction of as-received and deformed sheet specimens. Then, the performance of the modified Rousselier damage model in predicting forming behaviour, limiting strains, the onset of
instability, damage distribution and fracture geometry was investigated by comparing numerical results obtained from simulating uniaxial tension tests at different strain rates and quasi-static Marciniak tests, with experimental data.

The second step in this research was to design and develop a 3D cellular automata model in conjunction with the finite element constitutive model for multi-scale analysis of damage and fracture based on the model initially proposed by Shterenlikht [1]. Therefore, some micro-level material properties such as grain size were transferred and distributed across two different cell arrays assigned to capture ductile and brittle fracture behaviour of the material while the material model in the FE-model was used to represent macro-level strain gradients, stress states and macro-level damage behaviour. Each cell array assigned to each FE contains its unique understructural array of material properties determined by random number generators as a function of different distribution functions. Each ductile and brittle CA array follows independent criteria based on their different damage properties and nature but they interact with each other through a mapping function. In order to evaluate the performance of the hybrid FE+CA model, uniaxial tension tests and electrohydraulic free-forming (EHFF) tests were simulated using different process parameters (such as strain rate and temperature) and microstructural properties (such as grain size and martensite content) and the model outputs were compared to the experimental data obtained by different researchers [2][13]. The following sections conclude the main findings which were discussed in detail in their respective chapters, and provides recommendations for future research.

8.2 Conclusions

The following important conclusions can be drawn from the simulation of uniaxial tension tests, Marciniak tests and electrohydraulic free forming tests using the FE model and the hybrid FE+CA model:

- The combined non-linear regression with Markov chain Monte Carlo (NLR+MCMC) fitting procedure was found to be a powerful approach to successfully determine
hardening function parameters. The unique algorithm of NLR+MCMC which utilizes a target distribution as a stationary distribution instead of generating independent parameters make this parameter optimization method very efficient and accurate. Another advantage of this fitting procedure is that it can be used for a certain part of a function, e.g. fitting the strain-rate sensitive part in a multiplicative hardening model to a specific data set.

• Based on statistical analysis on the true stress-true strain flow curves and hardening rate, conducted on different types of constitutive hardening functions to evaluate the goodness of their fit, it was found that the multiplicative combination of the Voce-modified JC among saturated-type models and the modified Johnson-Cook among unbounded-type models exhibited the greatest accuracy although each one predicted the strain hardening rate behaviour differently at large strains.

• Since prediction of damage evolution along different strain paths depends on the approach in which a hardening function predicts the slope of the flow curve at strains beyond uniform elongation in uniaxial tension, obtaining extended work hardening flow curves at different strain rates, from low to high strain rates, can help the constitutive model to predict both the forming behaviour and the onset of localization more accurately.

• The Rousselier damage model is a continuous ductile damage model that can predict damage evolution even in zero or negative stress triaxiality. In its original form, the Rousselier constitutive model could successfully predict the strain distribution along the gauge area of DP600 tensile specimens at different strain rates, somehow independent of the hardening model, before the maximum load is reached. However, strain localization and damage evolution during post-uniform deformation, and final damage geometry showed strong sensitivity to the type of hardening model.

• The Rousselier damage model was modified by including strain-controlled void nucleation functions, void coalescence criteria and void growth acceleration functions. The predicted $f_c$ was in good agreement with the X-Ray tomography
analysis and reported in the literature for DP600. Based on the damage distribution map and final damage geometry of DP600 tensile specimens, predicted by the modified model, it is evident that using a void nucleation function and a void coalescence criterion with the Rousselier damage model are necessary for accurate predictions.

- Based on the calibration procedure used for the investigated DP600 sheet specimens, it was found that the Rousselier model constants ($D$ and $\sigma_1$ shown in Eq. 5.1b) were dependent on the type of hardening function if the original Rousselier model was employed. They were found to be $D = 2$ and $\sigma_1 = 450 \pm 5$ MPa for Voce-type functions, and $D = 2.5$ and $\sigma_1 = 390 \pm 15$ MPa for power law-type models. Nevertheless, the wide range of values for $D$ and $\sigma_1$ was considerably decreased by using the modified Rousselier damage model which includes secondary void nucleation and void coalescence criteria.

- Numerical simulation of Marciniak tests along three strain paths (UT, PS, and BT) showed that the modified Rousselier damage model can successfully predict the limiting strains that define the forming limit curve (FLC) of DP600 sheet.

- It was also shown that the damage evolution during the deformation is strongly strain-path dependent, but its sensitivity to the hardening model was significantly reduced when the modified Rousselier model used with strain controlled void nucleation function and void coalescence criterion.

- The dependency of the damage accumulation at the onset of necking (when maximum load was reached) and that of the final geometry of failure in each strain path to the hardening model, either saturated-type or unbounded-type, was considerably reduced when using the modified Rousselier model: both the accuracy and the consistency of the predictions were notably increased.

- The proposed hybrid finite element cellular automata (FE+CA) model is able to qualitatively (yet accurately) predict the fracture mechanism in terms of ductile and brittle fracture, by taking into account some microstructural properties of dual phase steels such as initial void volume fraction, grain size, grain orientation, and the martensite volume content.
Numerical simulations of uniaxial tension of fine- and coarse-grained DP600 and DP780 sheet specimens at strain rates of 1s\(^{-1}\) and 1000s\(^{-1}\) with the hybrid FE+CA model showed that greater ferrite grain sizes, higher martensite volume content, and higher strain rates would result in a considerable increase in the fraction of brittle fracture. It was shown that even in quasi-static uniaxial tension of DP780 sheet, the fracture mode transitioned from ductile fracture in an ultra-fined grained microstructure, to a mixture of ductile and brittle fracture mechanisms for fine-grained steel, and ultimately to brittle fracture for a coarse-grained material.

The FE+CA model is able to predict the occurrence of quasi-cleavage fracture in ultra-fine and fine-grained DP600 and DP780, as evidenced by a few brittle dead cells surrounded by ductile dead cells. It should be mentioned that the percentage of brittle fracture is used for qualitative comparison.

Parametric studies on the effect of temperature on the fraction of brittle fracture in uniaxial tension tests of DP780 sheet specimens at a strain rate of 1000s\(^{-1}\) showed that at \( T \approx 70^\circ \), the fracture mechanism would be approximately 50\% brittle.

At ambient temperature, the fracture behaviour at low and high strain rates do not change by increasing the grain size up to approximately 6\( \mu m \), however, the fraction of brittle fracture increases with higher rate at 1000s\(^{-1}\) compared to 1s\(^{-1}\).

Analysis of major and minor true strains in the simulation of 9.2kV and 10.3kV electrohydraulic free forming (EHFF) of fine-grained DP600 sheets showed that the model predicted a proportional equi-biaxial strain path for an element at the centre (i.e. near the apex) of the deformed specimen.

The damage geometry and fracture morphology was predicted accurately by the hybrid FE+CA model for the fine-grained (\( d_\gamma \approx 3 \mu m \)) DP600 sheets deformed under 13.6 kJ energy EHFF. Similar to the experiments, a negligible amount of brittle fracture was predicted although the strain rate reached approximately 2700s\(^{-1}\). Increasing the ferrite grain size to 12\( \mu m \) leads to a considerable increase.
in the percentage of brittle fracture. Thus, the ferrite grain size has a dominant influence on the fracture mechanism.

- One of the most important advantages of the proposed model is that it is a combination of a finite element constitutive model (to calculate macro-level strains, stresses and damage variables) and cellular automata (responsible for evaluating the fracture mode). Therefore, it is now possible to run parametric studies based on process parameters (such as strain path, strain rate, and temperature) and microstructural properties (such as grain size distribution, volume fraction and distribution of martensite) which can be very beneficial for steel producers.

8.3 Originality of the research

Firstly, a new optimization method based on a combination of non-linear regression (NLR) as the fitting procedure, and Markov chain Monte Carlo (MCMC)-Metropolis-Hastings (MH) algorithm as the optimization method, was proposed to calculate the coefficients of various types of hardening functions. This approach was shown to be both fast and more accurate than NLR alone. Subsequently, the effects of saturated- or unbounded-type hardening models, and of the slope of the flow curve at large strain levels on the Rousselier damage model were investigated for a wide range of strain rates.

Furthermore, the Rousselier damage model was extended to include a strain-controlled void nucleation function, a coalescence criterion and a void growth acceleration function. This modified version of the Rousselier damage model was developed for the first time and was found to be significantly more accurate than the original Rousselier model in predicting forming behaviour, damage accumulation and final fracture geometry of DP600 steel at various strain rates and for different strain paths.

Finally, the FE-scale micromechanical damage model was linked to a CA model which is capable of evaluating the ductile and brittle damage mechanisms using two corresponding CA arrays, and can take into account microstructural properties of
dual phase steels such as ferrite grain sizes, martensite content and grain orientations and their distributions along the specimen. Based on different distribution functions, sophisticated random number generators were implemented in the hybrid FE+CA model. This hybrid model was then employed for the first time to determine the dominant fracture mechanism and evaluate the effect of process parameters (such as strain rate and temperature) and microstructural features on the damage behaviour of DP600 and DP780 sheet specimens deformed in uniaxial tension and in electrohydraulic free forming (EHFF).

The numerical tools developed during this research were shown to be not only more accurate than existing models, but also offer new insights into the plastic deformation and damage development in multiphase sheet materials. These numerical tools can help steel suppliers improve the thermo-mechanical processing of dual or complex phase steels, which in turn will help to enhance the microstructure, and consequently, the mechanical properties and formability of these advanced high strength steel sheets. Moreover, because of the wide range of application of these numerical tools (i.e. these models are strain-rate and temperature-dependent), they are able to provide support for the development, optimization and industrial implementation of novel metal forming processes, such as electrohydraulic forming.

### 8.4 Future work recommendations

Based on the results and observations presented in this study, the following future investigations are recommended:

1. It is reported that the formability of sheet materials can be increased considerably at very high strain rates (greater than 15000s\(^{-1}\)) that are significantly above the range that was used to calibrate the hardening behaviour of the investigated DP600 sheet. Therefore, the accuracy of simulations will be improved if the extended flow curve of the desired alloys (beyond conventional uniaxial tension test limits) can be determined at the same levels of strain rate.
2. The modified Rousselier model was established based on isotropic hardening since the investigated DP600 did not show significant anisotropy. Including an anisotropic yield function such as Yld2004-18p or the Yoshida model (based on the second and third invariants of the deviatoric stress tensor) can make the proposed FE model more appropriate for anisotropic sheet materials subjected to different strain paths. Using a yield function with coefficients that are a function of strain and strain rate can also be used to study forming behaviour and optimize forming processes.

3. The developed model made it possible to investigate the evolution of the damage parameter in terms of void volume fraction. Therefore, conducting in-situ tension tests with high-resolution X-Ray micro-tomography may provide a better understanding of void evolution and validate the numerical results obtained by the proposed complete Rousselier damage model, with secondary void nucleation and void coalescence criteria.

4. The proposed hybrid FE+CA model is in its early stages. It can be used as the main platform for many future investigations. However, appropriate material characterisation as well as fracture analysis should be carried out so as to calibrate its parameters and size scales more precisely and validate its results. Furthermore, microstructural investigation by optical microscopy, quantitative fractography, SEM, TEM, and X-Ray tomography is suggested to identify the effect of the combination of process parameters such as strain path, strain rate and temperature with microstructural features such as the size of ferrite grains and their distribution, and the volume content, geometry and distribution of martensite on the fracture behaviour of dual phase steels.

5. Besides the distribution of microstructural features, the location of particular microstructural properties can be investigated with this model. In DP600, DP780 and DP980, martensite banding can be observed but no research has been reported so far to specifically identify the effect of banding on the failure behaviour of DP steels. The distribution of ferrite grain sizes and of martensite islands near the surface or at the mid-thickness of a DP sheet specimen can
be explored numerically and experimentally using this model and appropriate micro-scale characterizations.

6. The CA part of the code can be modified by implementing additional functions and parameters, e.g. taking into account the effect of bainite or retained austenite, and including the effect of thermal or adiabatic heating on damage behaviour of DP steels.

8.5 Bibliography


Rousselier Damage Model
Integration Procedure

The integration procedure of Rousselier continuum ductile damage model \[1, 3\] was carried out completely by Shterenlikht \[4\] for a single integration point. In this model, the plastic potential \((F)\) is written as:

\[
F = \frac{\sigma_{eq}}{\rho} - R(p) + B(\beta) D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right)
\]

where \(R(p)\) is the matrix flow behaviour of material hardening curve of material; \(\rho\) represents the dimensionless density, \(\sigma_1\) and \(D\) are the model parameters; \(B(\beta)\) is a damage function and is the conjugate force to the scalar damage variable \((\beta)\); \(\sigma_{eq}\) and \(\sigma_m\) denote the von Mises equivalent stress and the hydrostatic stress, respectively. The classical normality rule based on the plastic multiplier \((\lambda)\) or plastic strain increment \((\dot{\varepsilon}_p)\) can be written as:

\[
\dot{\varepsilon}^p = \lambda \frac{\partial F}{\partial (\sigma/\rho)}
\]

Accordingly:

\[
\dot{\varepsilon}_{ij}^p = \dot{p} \frac{3S_{ij}}{2\sigma_{eq}}
\]
\[
\dot{\varepsilon}_m^p = \dot{\varepsilon}_m B(\beta) D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right)
\]

\[
\dot{\sigma} = \dot{\varepsilon}_m
\]

\[
\dot{\beta} = \dot{\varepsilon}_D D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right)
\]

in which \( \dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^p - \dot{\varepsilon}_{ij}^m \delta_{ij} \) is the deviator of \( \dot{\varepsilon}^p \). It can be calculated that \( \dot{\sigma} = \dot{\varepsilon}_{eq}^p \). Thus, the internal hardening variable identifies with the cumulated equivalent plastic deformation.

By substituting finite differences instead of differentials, a complete set of functions and equations can be obtained:

\[
\Delta \varepsilon_m^p - \Delta \varepsilon_{eq}^p B(\beta) D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) = 0 \quad \text{(A.1)}
\]

\[
\frac{\sigma_{eq}}{\rho} - R(\varepsilon_{eq}^p) + B(\beta) D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) = 0 \quad \text{(A.2)}
\]

\[
B(\beta) = \frac{\sigma_1 f_0 \exp(\beta)}{1 - f_0 + f_0 \exp(\beta)} \quad \text{(A.3)}
\]

\[
\rho(\beta) = \frac{1}{1 - f_0 + f_0 \exp(\beta)} \quad \text{(A.4)}
\]

While the material behaves in a linear elastic way, \( \beta = 0 \). \( f_0 \) is the initial void volume fraction while \( f = B(\beta)/\sigma_1 \) can be considered as the current void volume fraction.
\[ \sigma_m = \sigma_m^e - 3K\Delta \varepsilon_{pm} \]  \hfill (A.5)
\[ \sigma_{eq} = \sigma_{eq}^e - 3G\Delta \varepsilon_{p eq} \]  \hfill (A.6)
\[ \Delta \beta = \Delta \varepsilon_{p eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \]  \hfill (A.7)

where

\[ \sigma_m^e = \frac{1}{3} \sigma_{ij}^e \]  \hfill (A.8)
\[ \sigma_{eq}^e = \sqrt{\frac{3}{2}} S_{ij}^e \sigma_{ij}^e \]  \hfill (A.9)
\[ S_{ij}^e = \sigma_{ij}^e - \sigma_m^e \delta_{ij} \]  \hfill (A.10)
\[ \sigma_{ij}^t = E_{ijkl} \hat{\varepsilon}_{kl} \]  \hfill (A.11)
\[ G = \frac{E}{2(1 + \nu)} \]  \hfill (A.12)
\[ K = \frac{E}{3(1 - 2\nu)} \]  \hfill (A.13)

\[ \hat{\varepsilon}_{kl}(t_{i+1}) = \varepsilon_{ij}^t(t_i) + \Delta \varepsilon_{ij} \]  \hfill (A.14)
\[ \varepsilon_{ij}^p(t_{i+1}) = \varepsilon_{eq}^p(t_i) + \Delta \varepsilon_{ij}^p \]  \hfill (A.15)
\[ \beta(t_{i+1}) = \beta(t_i) + \Delta \beta \]  \hfill (A.16)

During the calculations, \( t_{i+1} \) should be considered when the time is not mentioned explicitly.

Although Newton - Raphson’s method can be employed to solve Eq. A.1 to Eq. A.7, \( \Delta \varepsilon_{pm} \) and \( \Delta \varepsilon_{p eq} \) should be calculated by solving Eq. A.1 and Eq. A.2. If Eq. A.1 and Eq. A.2 are named \( f \) and \( g \) respectively, thus their related equations will be:

\[
\begin{align*}
f(\Delta \varepsilon_{pm}, \Delta \varepsilon_{p eq}, \Delta \beta) &= 0 \\
g(\Delta \varepsilon_{pm}, \Delta \varepsilon_{p eq}, \Delta \beta) &= 0
\end{align*}
\]  \hfill (A.17)
An iterative process should be employed to solve these two equations. In each cycle, the following matrix should be considered and solved:

\[ J \cdot c = Y \]  \hspace{1cm} (A.18)

where:

\[
J = \begin{bmatrix}
\frac{\partial f}{\partial \Delta \varepsilon_p^m} & \frac{\partial f}{\partial \Delta \varepsilon_p^{eq}} \\
\frac{\partial g}{\partial \Delta \varepsilon_p^m} & \frac{\partial g}{\partial \Delta \varepsilon_p^{eq}}
\end{bmatrix}
\]  \hspace{1cm} (A.19)

\[
c = \begin{bmatrix} c_m \\ c_{eq} \end{bmatrix}
\]  \hspace{1cm} (A.20)

\[
Y = -\begin{bmatrix} f \\ g \end{bmatrix}
\]  \hspace{1cm} (A.21)

Strain increments are updated in each cycle:

\[
\begin{align*}
\Delta \varepsilon_p^m(t_{i+1}) & \leftarrow \Delta \varepsilon_p^m(t_i) + c_m \\
\Delta \varepsilon_p^{eq}(t_{i+1}) & \leftarrow \Delta \varepsilon_p^{eq}(t_i) + c_{eq}
\end{align*}
\]  \hspace{1cm} (A.22)

and the components of the Jacobian can be determined as follows:
\[
\frac{\partial f}{\partial \Delta \varepsilon_m^p} = 1 - \frac{D \Delta \varepsilon_{eq}^p}{3\sigma_1} \frac{\partial}{\partial \Delta \varepsilon_m^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right]
\] (A.23)

\[
\frac{\partial f}{\partial \Delta \varepsilon_{eq}^p} = -\frac{B(\beta)}{3\sigma_1} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) - \frac{\Delta \varepsilon_{eq}^p D}{3\sigma_1} \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right]
\] (A.24)

\[
\frac{\partial g}{\partial \Delta \varepsilon_m^p} = \frac{\partial}{\partial \Delta \varepsilon_m^p} \left( \frac{\sigma_{eq}}{\rho} \right) + D \frac{\partial}{\partial \Delta \varepsilon_m^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right]
\] (A.25)

\[
\frac{\partial g}{\partial \Delta \varepsilon_{eq}^p} = \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left( \frac{\sigma_{eq}}{\rho} \right) - \frac{\partial R(\varepsilon_{eq}^p)}{\partial \Delta \varepsilon_{eq}^p} + D \frac{\partial}{\partial \Delta \varepsilon_m^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right]
\] (A.26)

The following terms should also be defined:

\[
\frac{\partial}{\partial \Delta \varepsilon_m^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] = \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_m^p} \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) + B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \left( \frac{1}{\sigma_1} \right) \left( \frac{\partial \sigma_m}{\partial \Delta \varepsilon_m^p} \frac{1}{\rho} + \sigma_m \frac{\partial^1 \rho}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_m^p} \right)
\] (A.28)

\[
\frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] = \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) + B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \left( \frac{1}{\sigma_1} \right) \left( \frac{\partial \sigma_m}{\partial \Delta \varepsilon_{eq}^p} \frac{1}{\rho} + \sigma_m \frac{\partial^1 \rho}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} \right)
\] (A.29)

\[
\frac{\partial}{\partial \Delta \varepsilon_m^p} \left( \frac{\sigma_{eq}}{\rho} \right) = \frac{\partial \sigma_{eq}}{\partial \varepsilon_m^p} \frac{1}{\rho} + \sigma_{eq} \frac{\partial^1 \rho}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_m^p}
\] (A.30)

\[
\frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left( \frac{\sigma_{eq}}{\rho} \right) = \frac{\partial \sigma_{eq}}{\partial \varepsilon_{eq}^p} \frac{1}{\rho} + \sigma_{eq} \frac{\partial^1 \rho}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p}
\] (A.31)
\( \frac{\partial B(\beta)}{\partial \beta} \) can be calculated from Eq. A.3:

\[
\frac{\partial B(\beta)}{\partial \beta} = \sigma_1 f_0 \frac{\exp(\beta)\left[1 - f_0 + f_0 \exp(\beta)\right] - f_0 \left[\exp(\beta)^2\right]}{\left[1 - f_0 + f_0 \exp(\beta)\right]^2}
\]

\[
\Rightarrow \frac{\partial B(\beta)}{\partial \beta} = \sigma_1 f_0 \frac{\exp(\beta)(1 - f_0) + f_0 \left[\exp(\beta)^2\right] - f_0 \left[\exp(\beta)^2\right]}{\left[1 - f_0 + f_0 \exp(\beta)\right]^2}
\]

\[
\Rightarrow \frac{\partial B(\beta)}{\partial \beta} = \frac{\sigma_1 f_0 \exp(\beta)(1 - f_0)}{\left[1 - f_0 + f_0 \exp(\beta)\right]^2}
\]

(A.32)

Also, other parameters can be determined as follows:

According to Eq. A.4 \[ \rightarrow \frac{\partial \rho}{\partial \beta} = f_0 \exp(\beta) \] (A.33)

According to Eq. A.5 \[ \rightarrow \begin{cases} 
\frac{\partial \sigma_m}{\partial \varepsilon^p_m} = -3K \\
\frac{\partial \sigma_m}{\partial \varepsilon^p_{eq}} = 0 
\end{cases} \] (A.34)

According to Eq. A.6 \[ \rightarrow \begin{cases} 
\frac{\partial \sigma_{eq}}{\partial \varepsilon^p_m} = 0 \\
\frac{\partial \sigma_{eq}}{\partial \varepsilon^p_{eq}} = -3G 
\end{cases} \] (A.35)

Calculating \( \frac{\partial \beta}{\partial \Delta \varepsilon^p_m} \) and \( \frac{\partial \beta}{\partial \Delta \varepsilon^p_{eq}} \) is somehow complicated due to the fact that \( \beta \), itself, is a function of \( \Delta \varepsilon^p_m \) and \( \Delta \varepsilon^p_{eq} \) according to Eq. A.7. Therefore, if Eq. A.7 is considered
as a function named $h$, the partial derivatives can be obtained as follows:

$$h(\Delta \beta, \Delta \varepsilon^p_m, \Delta \varepsilon^p_{eq}) = \Delta \beta - \Delta \varepsilon^p_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) = 0 \quad (A.36)$$

Using the formula for partial derivatives of an implicit function, the mentioned derivatives can be defined as:

$$\frac{\partial \beta}{\partial \Delta \varepsilon^p_m} = -\frac{\partial h}{\partial \Delta \varepsilon^p_m} \frac{\partial h}{\partial \Delta \beta} \quad (A.37)$$

$$\frac{\partial \beta}{\partial \Delta \varepsilon^p_{eq}} = -\frac{\partial h}{\partial \Delta \varepsilon^p_{eq}} \frac{\partial h}{\partial \Delta \beta} \quad (A.38)$$

Since $\beta = \beta_t + \Delta \beta$, it can be understood that:

$$\frac{\partial \beta}{\partial \Delta \varepsilon^p_m} = \frac{\partial \Delta \beta}{\partial \Delta \varepsilon^p_m}$$

$$\frac{\partial \beta}{\partial \Delta \varepsilon^p_{eq}} = \frac{\partial \Delta \beta}{\partial \Delta \varepsilon^p_{eq}}$$

$$\frac{\partial \frac{1}{\rho}}{\partial \Delta \beta} = \frac{\partial \frac{1}{\rho}}{\partial \beta}$$
Thus, according to Eq. A.36, Eq. A.37 and Eq. A.38:

\[
\begin{align*}
\frac{\partial h}{\partial \Delta \varepsilon_{eq}} & = - \Delta \varepsilon_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{1}{\rho \sigma_1} \frac{\partial \sigma_m}{\partial \Delta \varepsilon_{eq}} \\
\frac{\partial h}{\partial \Delta \varepsilon_{eq}} & = - D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) - \Delta \varepsilon_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{1}{\rho \sigma_1} \frac{\partial \sigma_m}{\partial \Delta \varepsilon_{eq}} \\
\frac{\partial h}{\partial \Delta \beta} & = 1 - \Delta \varepsilon_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{\sigma_m}{\sigma_1} \frac{1}{\rho} \frac{\partial \Delta \beta}{\partial \Delta \beta}
\end{align*}
\]

(A.39)

By substituting Eqs. A.39 in Eqs. A.37 and Eqs. A.38, the following terms can be obtained:

\[
\begin{align*}
\frac{\partial \beta}{\partial \Delta \varepsilon_{eq}} & = - \Delta \varepsilon_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{1}{\rho \sigma_1} \frac{\partial \sigma_m}{\partial \Delta \varepsilon_{eq}} - 3K \quad \text{(Eq. A.34)} \\
\frac{\partial \beta}{\partial \Delta \varepsilon_{eq}} & = -D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{1}{\rho \sigma_1} \frac{\partial \sigma_m}{\partial \Delta \varepsilon_{eq}} \\
\frac{\partial \beta}{\partial \Delta \beta} & = 1 - \Delta \varepsilon_{eq} D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{\sigma_m}{\sigma_1} \frac{1}{\rho} \frac{\partial \Delta \beta}{\partial \Delta \beta}
\end{align*}
\]

(A.40)

(A.41)
By substituting and combining Eqs. A.33 - A.35 with Eqs. A.28 - A.31 and Eqs. A.40 - A.41, the following terms can be calculated:

\[
\frac{\partial}{\partial \Delta \varepsilon_{p}} \left[ B(\beta) \exp \left( \frac{\sigma_{m}}{\rho \sigma_{1}} \right) \right] = \exp \left( \frac{\sigma_{m}}{\rho \sigma_{1}} \right) \left[ \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{p}} + \frac{B(\beta)}{\sigma_{1}} \left( \frac{\partial \sigma_{m}}{\partial \Delta \varepsilon_{p}} \frac{1}{\rho} + \sigma_{m} \frac{\partial^{1}}{\partial \rho} \frac{\partial \beta}{\partial \Delta \varepsilon_{p}} \right) \right] \tag{A.42}
\]

\[
\frac{\partial}{\partial \Delta \varepsilon_{eq}} \left[ B(\beta) \exp \left( \frac{\sigma_{m}}{\rho \sigma_{1}} \right) \right] = \exp \left( \frac{\sigma_{m}}{\rho \sigma_{1}} \right) \left[ \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}} + \frac{B(\beta)}{\sigma_{1}} \left( \frac{\partial \sigma_{m}}{\partial \Delta \varepsilon_{eq}} \frac{1}{\rho} + \sigma_{m} \frac{\partial^{1}}{\partial \rho} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}} \right) \right] \tag{A.43}
\]

\[
\frac{\partial}{\partial \Delta \varepsilon_{m}} \left( \frac{\sigma_{eq}}{\rho} \right) = \frac{\partial \sigma_{eq}}{\partial \varepsilon_{m}} \frac{1}{\rho} + \frac{\partial^{1}}{\partial \rho} \frac{\partial \sigma_{eq}}{\partial \Delta \varepsilon_{m}} \tag{A.44}
\]

\[
\frac{\partial}{\partial \Delta \varepsilon_{eq}} \left( \frac{\sigma_{eq}}{\rho} \right) = \frac{\partial \sigma_{eq}}{\partial \varepsilon_{eq}} \frac{1}{\rho} + \frac{\partial^{1}}{\partial \rho} \frac{\partial \sigma_{eq}}{\partial \Delta \varepsilon_{eq}} \tag{A.45}
\]

Finally, the components of the Jacobian and their derivatives can completely be defined:
\[
\frac{\partial f}{\partial \Delta \varepsilon_p} = 1 - \frac{D \Delta \varepsilon_{eq}}{3\sigma_1} \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] \tag{A.46}
\]

\[
\frac{\partial f}{\partial \Delta \varepsilon_{eq}^p} = - \frac{D}{3\sigma_1} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) - \Delta \varepsilon_{eq}^p \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] \right] \tag{A.47}
\]

\[
\frac{\partial g}{\partial \Delta \varepsilon_p} = \sigma_{eq} f_0 \exp(\beta) \frac{\partial \beta}{\partial \Delta \varepsilon_m^p} + D \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] \tag{A.48}
\]

\[
\frac{\partial g}{\partial \Delta \varepsilon_{eq}^p} = -\frac{3G}{\rho} + \sigma_{eq} f_0 \exp(\beta) \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} - \frac{\partial R(\varepsilon_p^p)}{\partial \Delta \varepsilon_{eq}^p} + D \frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] \tag{A.49}
\]

where:

\[
\frac{\partial}{\partial \Delta \varepsilon_m^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] = \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \left[ \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_m^p} + \frac{B(\beta)}{\sigma_1} \left( -\frac{3K}{\rho} + \sigma_m f_0 \exp(\beta) \frac{\partial \beta}{\partial \Delta \varepsilon_m^p} \right) \right] \tag{A.50}
\]

\[
\frac{\partial}{\partial \Delta \varepsilon_{eq}^p} \left[ B(\beta) \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \right] = \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \left[ \frac{\partial B(\beta)}{\partial \beta} \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} + \frac{B(\beta)}{\sigma_1} \sigma_m f_0 \exp(\beta) \frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} \right] \tag{A.51}
\]
where:

\[
\frac{\partial B(\beta)}{\partial \beta} = \frac{\sigma_1 f_0 \exp(\beta) (1 - f_0)}{[1 - f_0 + f_0 \exp(\beta)]^2} \tag{A.52}
\]

\[
\frac{\partial \beta}{\partial \Delta \varepsilon_{p_m}} = - \frac{-3K \Delta \varepsilon_{eq}^p \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right)}{\rho \left[ \sigma_1 - \Delta \varepsilon_{eq}^p \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \sigma_m f_0 \exp(\beta) \right]} \tag{A.53}
\]

\[
\frac{\partial \beta}{\partial \Delta \varepsilon_{eq}^p} = - \frac{D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{\sigma_m}{\sigma_1} f_0 \exp(\beta)}{1 - \Delta \varepsilon_{eq}^p D \exp \left( \frac{\sigma_m}{\rho \sigma_1} \right) \frac{\sigma_m}{\sigma_1} f_0 \exp(\beta)} \tag{A.54}
\]

Equations A.1-A.22 are needed to calculate \( \Delta \varepsilon_{p_m} \) and \( \Delta \varepsilon_{eq}^p \). Once they are obtained, \( \sigma_m \) and \( \sigma_{eq} \) can be found from Eq. A.3 and Eq. A.6, and \( \beta \) can be calculated by using Eq. A.16 and Eq. A.7 and

\[
\begin{aligned}
\sigma_{ij} &= \sigma_{eq} + \sigma_m \delta_{ij} \\
\Delta \varepsilon_{eq}^p &= \frac{3}{2} \frac{S_{eq}}{S_{eq}} \Delta \varepsilon_{eq} + \Delta \varepsilon_{m} \delta_{ij} \\
\varepsilon_{ij}^e &= \varepsilon_{ij}^e(t_i) + \Delta \varepsilon_{ij} - \Delta \varepsilon_{ij}^p
\end{aligned} \tag{A.55}
\]

It is also noteworthy that according to Eqs. A.14-A.16, the elastic strain tensor (\( \hat{\varepsilon}_{kl} \)), equivalent plastic strain (\( \varepsilon_{eq}^p \)) and the damage variable (\( \beta \)) should be stored from one time increment to another throughout the analysis.
A.1 Bibliography


Non-linear Regression

The process of finding the equation of the curve of best fit, which may be most suitable for predicting the unknown values, is known as curve fitting. Therefore, curve fitting means an exact relationship between two variables by algebraic equations. The following methods are utilized for fitting a curve [1].

1. Graphic method
2. Method of group average
3. Method of moments
4. Principle of least squares

Out of above four methods, only the principle of least squares is discussed and presented here. The principle of least squares provides a unique set of values to the constants and hence suggests a curve of best fit to the given data. The method of least squares is probably the most systematic procedure to fit a unique curve through a given set of data points.

The method of least squares is a standard approach to the approximate solution of overdetermined systems, i.e., sets of equations in which there are more equations than
unknowns. "Least squares" means that the overall solution minimizes the sum of the squares of the errors made in the results of every single equation. In the least squares method, the one curve which provides the minimum error is then the ‘best’ curve.

**Nonlinear regression** uses a computationally intensive, iterative approach that can only be explained using calculus and matrix algebra. The method requires initial estimated values for each parameter \[1\]. The following Functions can be used for linear regression either directly or by taking logarithm of both sides:

- Any form of polynomials
  
  \[ f(x) = ax^n + bx^{n-1} + cx^{n-2} + \ldots \]

  \[ f(x,y) = ax^n y^m + bx^{n-1} y^{m-1} + cx^{n-2} y^{n-2} + \ldots \]

- power-laws
  
  \[ f(x) = ax^n \]

- exponential functions
  
  \[ f(x) = a \exp(bx) \]

The general expression for any error using the least squares approach is

\[
\text{error} = \sum_{n=1}^{n} (d_n)^2 = \sum_{n=1}^{n} (y_n - f(x_n))^2
\]

where \(y_n\) is observed value. If the proposed function \(f(x)\) has coefficients \(c_i\), The error then can be minimized when:

\[
\frac{\partial \text{error}}{\partial c_i} = \sum_{n=1}^{n} \frac{\partial (y_n - f(x_n))^2}{\partial c_i} = 0
\]

Consider a set of stress - strain data which has \(n\) points. If one wants to fit Holloman’s law (power-law) to that dataset:
\[ \sigma(\varepsilon) = k \varepsilon^n \quad \text{(B.3)} \]

\[ \ln(\sigma) = \ln k + n \ln(\varepsilon) \quad \text{(B.4)} \]

\[ \ln(\sigma) = Y, \ \ln k = K, \ \ln(\varepsilon) = X \quad \text{(B.5)} \]

\[ Y = nX + K \quad \text{(B.6)} \]

\[ \text{error} = \sum_{i=1}^{m} (Y_i - (K + nX_i))^2 \quad \text{(B.7)} \]

and to find the minimum of error function, the derivative of the error with respect to \( n \) and \( K \) should be taken and set each to zero:

\[ \frac{\partial \text{error}}{\partial n} = -2 \sum_{i=1}^{m} X_i (Y_i - (K + nX_i)) = 0 \quad \text{(B.8)} \]

\[ \frac{\partial \text{error}}{\partial K} = -2 \sum_{i=1}^{m} (Y_i - (K + nX_i)) = 0 \quad \text{(B.9)} \]

Rewriting the above equations:

\[ \sum_{i=1}^{m} X_i Y_i = K \sum_{i=1}^{m} X_i + n \sum_{i=1}^{m} X_i^2 \quad \text{(B.10)} \]

\[ \sum_{i=1}^{m} Y_i = K \sum_{i=1}^{m} 1 + n \sum_{i=1}^{m} X_i \quad \text{(B.11)} \]

By writing them in matrix form:

\[ A = \begin{bmatrix} \sum_{i=1}^{m} X_i & \sum_{i=1}^{m} X_i^2 \\ m & \sum_{i=1}^{m} X_i \end{bmatrix} \quad \text{(B.12)} \]

\[ Z = \begin{bmatrix} n \\ K \end{bmatrix} \quad \text{(B.13)} \]
Finally:

\[ A \cdot Z = B \Rightarrow Z = A^{-1} \cdot B \]  

(B.15)

For non-linear regression, i.e. the function is non-linear based on coefficients, the Newton-Raphson method should be utilized to solve a system of nonlinear equations. Consider the solution to a system of \( n \) non-linear equations in \( n \) unknowns given by [2, 3]:

\[
\begin{align*}
    f_1(c_1, c_2, \ldots, c_n) &= 0 \\
    f_2(c_1, c_2, \ldots, c_n) &= 0 \\
    \vdots \\
    f_n(c_1, c_2, \ldots, c_n) &= 0
\end{align*}
\]

(B.16)

These equations can be the minimization equations, like eq. 11 or eq. 17, eq. 18 in which \( c_i \) are the coefficients. The system can be written in a single expression using vectors, i.e.,

\[ f(C) = 0 \]

where vector \( C \) contains the independent variables, and vector \( f \) contains the functions \( f_i(C) \):

\[
C = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}, \quad f(C) = \begin{bmatrix} f_1(c_1, c_2, \ldots, c_n) = 0 \\ f_2(c_1, c_2, \ldots, c_n) = 0 \\ \vdots \\ f_n(c_1, c_2, \ldots, c_n) = 0 \end{bmatrix} = \begin{bmatrix} f_1(C) \\ f_2(C) \\ \vdots \\ f_n(C) \end{bmatrix}
\]

(B.17)

A Newton-Raphson method for solving the system of equations requires the evaluation of a matrix, known as the **Jacobian** of the system, which is defined as:
\[ J = \frac{\partial(f_1, f_2, \ldots, f_n)}{\partial(c_1, c_2, \ldots, c_3)} = \begin{bmatrix} \frac{\partial f_1}{\partial c_1} & \frac{\partial f_1}{\partial c_2} & \cdots & \frac{\partial f_1}{\partial c_n} \\ \frac{\partial f_2}{\partial c_1} & \frac{\partial f_2}{\partial c_2} & \cdots & \frac{\partial f_2}{\partial c_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial c_1} & \frac{\partial f_n}{\partial c_2} & \cdots & \frac{\partial f_n}{\partial c_n} \end{bmatrix} \] (B.18)

If \( c = c_0 \) (a vector) represents the first guess for the solution, successive approximations to the solution are obtained from:

\[ c_{n+1} = c_n - J^{-1} f(c_n) = c_n - \Delta c_n \] (B.19)

A convergence criterion for the solution of a system of non-linear equations could be, for example, the difference between consecutive values of the solution, i.e.,

\[ \max |(c_i)_{n+1} - (c_i)_n| < \epsilon \]

or,

\[ |\Delta c_n| = |c_{n+1} - c_n| < \epsilon \]

The main difficulty with using Newton-Raphson to solve a system of non-linear equations is having to define all the functions \( \frac{\partial f_i}{\partial c_i} \), for \( i, j = 1, 2, \ldots, n \) included in the Jacobian. As the number of equations and unknowns, \( n \), increases, so does the number of elements in the Jacobian, \( n^2 \).
B.1 Bibliography


Appendix C

Material properties in ABAQUS

Table C.1 shows the properties that need to be provided to ABAQUS finite element simulation software to run a simulation based on the hybrid FE+CA model. It is worth noting that the first 15 items are needed for FE-scale model and properties 16–33 are needed for CA-scale part of the model. In addition, if a material name for a particular part of the model geometry starts with "cafe", full hybrid FE+CA model will be used for the explicit FE analysis of the elements associated with that particular part. Otherwise, only FE-scale model (the Rousselier damage model with hardening functions, void nucleation functions and void coalescence criteria) will be used for FE-scale analysis, as shown in Fig. C.1. This is especially important to reduce computational cost and utilize the FE+CA model for a specific part of the specimen in which the damage is more likely to occur.

Table C.1: List of material properties needs to be fed in ABAQUS

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<th>No.</th>
<th>Property name</th>
<th>Description</th>
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<tr>
<td>1</td>
<td>E</td>
<td>Young’s modulus</td>
</tr>
<tr>
<td>2</td>
<td>nu</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>3</td>
<td>D</td>
<td>Rousselier damage variable</td>
</tr>
<tr>
<td>4</td>
<td>void_nuc_select</td>
<td>Void nucleation function case selector</td>
</tr>
<tr>
<td>5</td>
<td>sig1</td>
<td>Rousselier damage variable</td>
</tr>
<tr>
<td>6</td>
<td>void_coal_select</td>
<td>Void coalescence criteria case selector</td>
</tr>
<tr>
<td>7</td>
<td>hard_selec</td>
<td>Hardening function case selector</td>
</tr>
</tbody>
</table>

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<th>No.</th>
<th>Property name</th>
<th>Description</th>
</tr>
</thead>
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<td>C1</td>
<td>Hardening function parameter</td>
</tr>
<tr>
<td>9</td>
<td>C2</td>
<td>Hardening function parameter</td>
</tr>
<tr>
<td>10</td>
<td>C3</td>
<td>Hardening function parameter</td>
</tr>
<tr>
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<td>C4</td>
<td>Hardening function parameter</td>
</tr>
<tr>
<td>12</td>
<td>C5</td>
<td>Hardening function parameter</td>
</tr>
<tr>
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<td>C6</td>
<td>Hardening function parameter</td>
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<td>C7</td>
<td>Hardening function parameter</td>
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<tr>
<td>15</td>
<td>C8</td>
<td>Hardening function parameter</td>
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<tr>
<td>16</td>
<td>nc</td>
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</tr>
<tr>
<td>17</td>
<td>ncb</td>
<td>Number of brittle cells per array dimension</td>
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<td>18</td>
<td>bfm</td>
<td>Mean scalar damage variable</td>
</tr>
<tr>
<td>19</td>
<td>bfmstd</td>
<td>Standard deviation of scalar damage variable</td>
</tr>
<tr>
<td>20</td>
<td>wbetl</td>
<td>Weibull distribution parameter for small grain sizes</td>
</tr>
<tr>
<td>21</td>
<td>wetal</td>
<td>Shape parameter of Weibull distribution for small grain sizes</td>
</tr>
<tr>
<td>22</td>
<td>wgaml</td>
<td>Scale parameter of Weibull distribution for small grain sizes</td>
</tr>
<tr>
<td>23</td>
<td>wbetr</td>
<td>Weibull distribution parameter for larger grain sizes</td>
</tr>
<tr>
<td>24</td>
<td>wetar</td>
<td>Shape parameter of Weibull distribution larger grain sizes</td>
</tr>
<tr>
<td>25</td>
<td>wgamr</td>
<td>Scale parameter of Weibull distribution larger grain sizes</td>
</tr>
<tr>
<td>26</td>
<td>wlwr</td>
<td>The ratio of larger grain sizes to small grain sizes</td>
</tr>
<tr>
<td>27</td>
<td>gammmap</td>
<td>Effective surface energy</td>
</tr>
<tr>
<td>28</td>
<td>dscc</td>
<td>Strain concentration constant for ductile cells</td>
</tr>
<tr>
<td>29</td>
<td>bscinc</td>
<td>Strain concentration constant for brittle cells</td>
</tr>
<tr>
<td>30</td>
<td>part</td>
<td>Fraction of brittle cells that have an adjacent cracked carbide</td>
</tr>
<tr>
<td>31</td>
<td>maxmis</td>
<td>Maximum possible misorientation angle in degrees</td>
</tr>
<tr>
<td>32</td>
<td>misor_ther</td>
<td>Misorientation threshold in degrees</td>
</tr>
<tr>
<td>33</td>
<td>path_select</td>
<td>Path to save the results (for Linux and Windows computers)</td>
</tr>
</tbody>
</table>
Figure C.1: Material definition and properties used in ABAQUS FE simulation software
Recommended material parameters

Throughout this research, various functions, equations and criteria such as damage models, hardening functions, void nucleation models and void coalescence criteria were introduced and evaluated. The following functions and parameters are recommended as the mechanical and materials properties of DP600 sheet specimens when using commercial finite element software (e.g. ABAQUS):

- general mechanical properties of as received DP600

Table D.1: Mechanical properties of as-received DP600 sheet

<table>
<thead>
<tr>
<th>Parameters</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\rho$ (kg/m$^3$)</th>
<th>$\sigma_y$ (MPa)</th>
<th>$\sigma_{UTS}$ (MPa)</th>
<th>$\epsilon_{UTS}$ (%)</th>
<th>$\epsilon_t$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values</td>
<td>206</td>
<td>0.3</td>
<td>7800</td>
<td>375</td>
<td>617</td>
<td>17.4</td>
<td>25.5</td>
</tr>
</tbody>
</table>

- among strain-dependent hardening models: the 4-parameter Voce model (Eq. 6.3c)

Table D.2: Hardening parameters calculated DP600 sheet

<table>
<thead>
<tr>
<th></th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voce (4-parameter)</td>
<td>369.13</td>
<td>712.49</td>
<td>13.971</td>
<td>331.84</td>
</tr>
</tbody>
</table>
• among rate-dependent hardening models: the multiplicative combination of 3-parameter Voce and modified JC (Eq. 4.5e), and the modified JC model (Eq. 4.4) as saturated-type and unbounded-type flow hardening functions

Table D.3: Coefficients of hardening functions for DP600

<table>
<thead>
<tr>
<th></th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>modified JC (mJC)</td>
<td>225.35</td>
<td>850.16</td>
<td>0.3194</td>
<td>0.0037</td>
<td>1.5715</td>
</tr>
<tr>
<td>Voce-mJC (VmJC)</td>
<td>400.21</td>
<td>795.19</td>
<td>9.0236</td>
<td>0.0015</td>
<td>1.9430</td>
</tr>
</tbody>
</table>

• The Rousselier damage model parameters and the strain-controlled void nucleation function (Eq. 6.4) to take into account secondary void nucleation in DP600

Table D.4: Rousselier damage parameters for DP600

<table>
<thead>
<tr>
<th>$D$</th>
<th>$\sigma_k$ (MPa)</th>
<th>$f_N$</th>
<th>$\varepsilon_N$</th>
<th>$S_N$</th>
<th>$f_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>425</td>
<td>0.02</td>
<td>0.35</td>
<td>0.11</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The mechanical properties required as input in the FE model can be determined from mechanical tests such as uniaxial tension tests. The FE-model can be used independently of the CA-model for forming process optimization and parametric studies based on different strain paths, strain rates and temperatures. On the other hand, the microstructural properties needed for the CA-model, i.e. distribution and location of microstructural features such as ferrite grain size and martensite volume fraction, can be obtained by material characterization and metallography. The size of the damage cells should be chosen between 0.1 – 0.5 mm and 0.005 – 0.05 mm and 0.005 – 0.05 mm (typically 10 – 20 times larger than the mean (or median) grain size) for the ductile and brittle cell arrays, respectively. Then, based on Eq. 3.1 and Eq. 3.3, the total number of cells in each CA array and the size of finite elements can be determined.
D.1 Bibliography


Appendix E

Complementary FE-model information

The proposed hybrid FE+CA model was developed based on explicit solution of dynamic equilibrium since one of the objectives of this research was to evaluate the forming and damage behaviour as well as final failure geometry of dual phase steels under a wide range of forming processes, from quasi-static conditions to high strain rates, with various contact conditions. Due to the dynamic nature of high strain rate forming processes (such as EHF), explicit solution was considered as the appropriate choice. It was then implemented as a user material subroutine for use in the Abaqus/Explicit finite element software.

A mesh sensitivity analysis was carried out by reducing the element size from 1 mm to 0.065 mm for quasi-static specimens to determine the effect of element size on the simulation of tensile tests and performance of the FE model. Detailed description of the simulation procedure is described in Section 4.3.4. Based on Fig. E.1 simulation results in terms of load versus displacement showed good consistency for an element size less than 0.25 mm in the damaged area and acceptable accuracy and computational cost, for quasi-static. Therefore, biased meshing, ranging from 0.5 mm near the grip section to 0.2 mm near the middle of the gauge length, was used for quasi-static deformation. A similar procedure was used to determine the mesh size for the miniature dog-bone
In order to decrease computation costs, mass scaling was used to increase the time step by scaling up the density of specific elements that control the time step due to their size. The user specifies a minimum time step at the beginning of the simulation. And the density of elements that have a time step smaller than this minimum value is increased to the point where the corresponding time step is equal to the minimum time step. Mass scaling is widely used to reduce simulation times in quasi-static analyses where the velocity is low, and the kinetic energy is small compared to the internal energy. To ensure the quasi-static condition, kinetic energy should not exceed 10% of the internal energy. Figure E.2 shows the evolution of internal and kinetic energy as a function of time for uniaxial tension tests at 0.1 and 1 s\(^{-1}\) and Marciniak tests. It can be seen that the fraction of the kinetic energy compared to internal energy is negligible in all cases.

In order to confirm the accuracy of the proposed hardening equations and the ability of the Rousselier model to predict the strain distribution along the gauge area, the average level of plastic strain in the neck and in the uniform deformation area are compared in Fig. E.3. It can be seen from Fig. 4.14 and Fig. E.3 that all models are successfully able to calculate the strain distribution since the predicted results lie within 1\(\sigma\) (one standard deviation) of the DIC results derived from experimental tests.
It is also worth noting that Voce–combination hardening models predict a lower level of average strain both inside and outside the neck at all strain rates which means that these functions predict a lower uniform deformation, more strain localization as well as a higher gradient of deformation across the neck. Comparing with experiments, some variation can be observed especially for the Voce–type hardening models which seem to underestimate the strain in those sections. However, it can be understood that after the time when maximum load is reached and prior to the occurrence of a localized neck, the geometry of the neck, the strain in the centre of the neck, and the strain distribution in the uniformly deformed area and in the necking section are approximately independent of the hardening model that is employed.
Figure E.3: Comparison of experimental and calculated average strain in (a) the uniformly deformed gauge area and (b) in the neck for DP600.
Appendix F

References to experimental procedures and results

A detailed description of the testing procedures, specimens, tools and apparatus, measurement procedures and obtained experimental results can be found in the following references:

- **Chapter 4.5**: uniaxial tension tests at low, intermediate and high strain rates:


- **Chapter 6**: Marciniak tests, extended flow curve, strain measurements and techniques:

  
  

- **Chapter 7**: materials characterization, metallography and fractography:

  
  
  
  
Chapter 7: electrohydraulic forming (EHF):


VITA AUCTORIS

NAME: Iman Sari Sarraf

PLACE OF BIRTH: Tehran, Iran

YEAR OF BIRTH: 1983

EDUCATION:

Bachelor of Science (BSc)
Materials Science and Engineering
Iran University of Science and Technology
Tehran, Iran
2006

Master of Science (MSc)
Materials Science and Engineering–Metal Forming
Sharif University of Technology
Tehran, Iran
2009

Philosophy Degree (PhD)
Engineering Materials
University of Windsor
Windsor, Canada
2017