**Modeling of Deformation in Ideal Plastic
Material with Evolving Porosity**

by

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B. Eng. (Mechanical Engineering)

A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfillment of the requirements
for the degree of

Masters of Engineering
in Mechanical Engineering

**Department of Mechanical and Aerospace Engineering
Ottawa-Carleton Institute
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Modeling of Deformation in Ideal Plastic Material with Evolving Porosity

submitted by

Steven Ralph Lawrence Amond
B. Eng. (Mechanical Engineering)

in partial fulfillment of the requirements
for the degree of Masters of Engineering
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Thesis Supervisor

Chair, Department of Mechanical and Aerospace Engineering

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Abstract

The study of fracture mechanics has resulted in increased understanding of the mechanisms involved in fracture processes of materials. From the original linear approximations for stress around the crack tip, through the corrections to these models to account for nonlinearities, to the present models that account for microstructural interactions, such as void initiation, growth and coalescence, fracture analysis has become increasingly better at predicting this complex behaviour. A recent constitutive model, developed by Ponte Castaneda and Zaidman, the PCZ model, predicts the effective behaviour of porous material by accounting for the evolution of the void fraction and aspect ratio. Including the aspect ratio leads to a competition between its effects on the hardening rate of the material and the same effect introduced by the void fraction.

The research for this graduate program comprised the implementation of the PCZ model as a constitutive relation in an object oriented code simulating various manufacturing processes. The resulting code was subsequently used to conduct tests to examine the effects of: Poisson's Ratio, initial stress, initial prescribed void type and cyclic loading, on the results predicted by the PCZ model.

It was found that the PCZ model produces expectable results under the uniaxial loading conditions examined. Under cyclic loading conditions void coalescence and collapse were observed for spheroidal and spherical voids respectively. This observation was the same regardless of whether tensile or compressive average strain levels were present.

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Nomenclature

a	Void semi-axis length in the major loading direction.
$A_{ijk}^{(2)}$	Strain Intensity tensor.
b	Void semi-axis length in the minor loading direction.
B	Matrix used to map the average stress in the porous material to the derivative of the effective yield function with respect to average stress.
c	Void semi-axis length in the minor loading direction.
$\overline{D}_{ij}$	Average strain-rate over the domain of the porous material.
E	Young's Modulus.
f	Void volume fraction.
$\dot{f}$	Time rate of change of the void volume fraction.
H	Rate of hardening in the porous material.
$\dot{K}$	Mapping between the average stress rate and the average strain rate in the porous material. Referred to as the "dynamic stiffness matrix".
$\dot{K}^+$	Pseudo inverse of the dynamic stiffness matrix.
$l_i (i = 1,3)$	Semi-axis lengths of general ellipsoidal voids in the porous material.
$L_i (i = 1,3)$	Spacings between general ellipsoidal voids in the porous material.
$\tilde{L}$	Estimate for the effective viscosity tensor of a linear composite.
$\hat{L}^{(r)}$	Viscosity tensor of the rth phase in the linear composite.

$L^{(0)}$	Viscosity tensor for a homogeneous comparison material.
Q^2	Function of average stress, void fraction and aspect ratio. Used in the relation for the effective yield function.
S_{ijkl}	Eshelby tensor.
$\tilde{U}$	Effective stress potential of the porous material.
w, w_1, w_2	Aspect ratio of the voids in the porous material and their spacings.
$\dot{w}_1, \dot{w}_2$	Time rate of change of the void aspect ratios
$\tilde{\phi}$	Effective yield function of the porous material.
ν_{matrix}	Poisson's ratio of the matrix phase in the porous material.
$\bar{\sigma}_{ij}$	Average stress tensor over the domain of the porous material.
$\dot{\bar{\sigma}}_{ij}$	Average stress-rate in the porous material.
σ_y	Yield stress of the matrix phase in the porous material.
$\bar{\sigma}_m$	Hydrostatic stress in the porous material.
$\bar{\sigma}_e$	Equivalent stress of the porous material in terms of the deviatoric stress.
σ'	Deviatoric stress in the porous material.

Chapter 1

1.0 Introduction

Fractures or failures of various forms have occurred throughout history and effected a vast number of individuals. For this reason engineers and scientists have introduced a field of study that is concerned primarily with the mechanisms involved in the failure of various materials. The study of fracture mechanics allows possible failure scenarios to be predicted in the design stage and hopefully avoided in service. During the development of the basic concepts of fracture mechanics, early researchers were generally restricted to materials that obeyed Hookean models. In some instances they did introduce small corrections to account for nonlinearities, such as plasticity, however, these models still assumed that the global behaviour of the structure remained linear-elastic. Eventually, theories were developed to deal with several types of non-linear material behaviours such as plasticity, viscoplasticity and viscoelasticity. Although these theories included advanced fracture concepts, they were merely extensions of Linear Elastic Fracture Mechanics (LEFM). In addition, the models developed, both linear and nonlinear, assumed that the structure of the material essentially remained fixed. No attempts were made to introduce parameters to account for

evolving microstructure, a phenomenon that is observed during most deformation processes. One particular example of evolution is seen in the tensile loading of ductile materials. In this instance many microstructural changes are observed, but of particular interest in the analysis of failure are: void nucleation, growth and coalescence. These microstructural changes modify the behaviour of the material markedly and should be included in failure analysis. As a result, more recently, researchers have focused their efforts on developing material models that specifically account for these evolutions. These models fall into three main categories: finite shell models, periodic microstructure models and variational principle models. The model used in the present thesis involves a combination of the last two methods. As a precursor to the presentation of this work, the remainder of this chapter will briefly outline the major contributions in the development of fracture theories from the initial elastic models to those with evolving microstructure.

1.1 Linear Fracture Analysis Models

From an atomic point of view, fracture of materials occurs when an externally applied stress is sufficient to break the bonds that hold atoms together. From Figure 1.1 it can be seen that a tensile force is required to increase the inter-atomic spacing from that of the equilibrium spacing, x_0 . To

completely sever the bond, this force must be in excess of the cohesive force. A resulting estimate of the cohesive strength is:

$$\sigma_c = E/\pi \quad (1.1)$$

where E is Young's Modulus. Experimental fracture strengths, however, are typically much lower than this estimate. This is due to many factors, one being that this simplified model assumes that all the bonds, on any given plane, will be broken simultaneously, which in reality is not the case. For example, during ductile fracture, localized plastic flow occurs leading to necking and eventual component failure. However, an even more intrinsic cause for the lower cohesive strengths can be derived from the work of Leonardo da Vinci, who measured qualitatively the strengths of iron wires and found that they varied inversely with wire length. Since the number of flaws in each wire is directly related to its length, this result implies that flaws in the material control the strength. Recalling that fracture will only occur when the stress at the atomic level exceeds the cohesive strength of the material it can be concluded that the flaws lower global strength by magnifying the stress locally.

The first investigator to qualitatively examine this stress concentration effect was Inglis [1] who examined elliptical holes in flat plates. His analysis included an elliptical hole in an infinitely large plate subjected to an applied load, Figure 1.2. As the major axis is increased the elliptical hole begins to take

on the appearance of a sharp crack. For the case when $a \gg b$, Inglis defined the stress at the tip of the major axis, point A, in terms of the radius of curvature, ρ :

$$\sigma_A = 2\sigma\sqrt{a/\rho} \quad (1.2)$$

where σ is a uniaxial stress perpendicular to the major axis of the elliptical hole. Subsequent researchers have shown that the stress field in any linear elastic cracked body can be given by (Figure 1.3):

$$\sigma_y = (k/\sqrt{r})f_y(\theta) + \text{other terms} \quad (1.3)$$

where σ_y is the stress tensor, r and θ are defined in Figure 1.3, k is a coefficient, f_y is a dimensionless function of θ and the subsequent terms are related to the geometry of the system. The leading term in Equation 1.3, approaches infinity as r tends to zero, thus Equation 1.3 describes a stress singularity. There are three main types of loading that can be applied to a crack, see Figure 1.4. The cracked body can be loaded in any one of these modes or any combination of the three. Each loading mode produces the crack tip singularity described by Equation 1.3, but the coefficient, k , and function, f_y , depend on the mode. For this reason k is replaced by $\frac{K}{\sqrt{2\pi}}$ where the stress intensity factor, K , as yet undetermined, is usually given a

subscript to denote the mode of loading, i.e. K_I , K_{II} or K_{III} . With this change, the stress fields ahead of the crack tip in an isotropic linear elastic material can be written as:

$$\lim_{r \rightarrow 0} \sigma_y^{(I)} = (K_I / \sqrt{2\pi r}) f_y^{(I)}(\theta) \quad (1.4a)$$

$$\lim_{r \rightarrow 0} \sigma_y^{(II)} = (K_{II} / \sqrt{2\pi r}) f_y^{(II)}(\theta) \quad (1.4b)$$

$$\lim_{r \rightarrow 0} \sigma_y^{(III)} = (K_{III} / \sqrt{2\pi r}) f_y^{(III)}(\theta) \quad (1.4c)$$

for the three modes respectively. In a mixed mode problem the principle of linear superposition may be employed to determine the various stress components. A detailed collection of expressions for the stress components as well as displacements for the three modes can be found in Tables 1.1-1.3.

It should be noted that the equations outlined in Tables 1.1-1.3 describe the crack tip fields in only a small volume around the crack tip defined as the singularity dominated zone. The stresses outside this zone are governed by the remote boundary conditions, see Figure 1.5. For this reason, K is a very important parameter in fracture mechanics because it completely defines the crack tip conditions i.e. if known, then K can be used to solve for all components of stress, strain and displacement.

The linear model of Inglis, Equation 1.2, predicts an infinite stress at the tip of an infinitely sharp crack, $\rho = 0$. This caused some concern since no material can withstand infinite stress. This concern motivated Griffith [2] to

develop a fracture theory based on energy rather than local stress. The results of Griffith's work produced an alternate derivation of the stress intensity factor, making it one of the fundamental models of fracture mechanics.

With reference to the first law of thermodynamics which states that, when a system goes from a non equilibrium state to equilibrium there will be a net decrease in energy, Griffith proposed a theory for the formation, or growth, of a crack. Griffith postulated that a crack can form, or an existing crack can grow, only if such a process causes the total energy to decrease or remain constant. Thus, the critical condition for fracture was defined as: the point where crack growth occurs, under equilibrium conditions, with no net change in total energy. Griffith developed this theory for elastic materials based on an energy balance between (1) the surface energy of a crack and (2) the stored internal elastic energy. In order to develop expressions for these quantities Griffith considered an elliptical hole in an infinite plate with thickness, t (Figure 1.6). The energy balance produced a criterion for crack growth:

$$2\gamma_s = \pi\sigma^2 a/E \quad (1.5)$$

where

- a - half the crack length
- γ_s - specific surface energy
- σ - stress
- E - Young's Modulus

Solving Equation 1.5 for $a = a_c$, the critical crack length for σ gives:

$$a_c = 2\gamma_c E / \sigma^2 \pi \quad (1.6)$$

Rearrange Equation 1.5, with the material constants on one side and the terms related to the stress field and crack geometry on the other, the following is attained [3]:

$$K = \sigma \sqrt{\pi a} \quad (1.7)$$

where the stress intensity factor $K = \sqrt{2\gamma_c E}$. Note that this result is for an elliptical hole in an infinite plate under Mode I loading. For any other crack K can be related to Equation 1.7 through an appropriate correction factor:

$$K_{(I, II, or III)} = C \sigma \sqrt{\pi a} \quad (1.8)$$

where C is a dimensionless constant that depends on geometry and mode of loading.

1.2 Nonlinear Fracture Analysis Models

The stress concentration model proposed by Inglis predicted infinite stress at the crack tip. This behaviour does not occur in real materials because inelastic material deformations, such as plasticity, take place at the crack tip, leading to a decrease in stress in this region. If the crack tip yielding is moderate i.e. small compared to the overall dimensions, then simple corrections to the stress intensity factor can be applied to account for these inelastic crack tip behaviours. This section will present models that were developed to produce these corrections.

Irwin[6] observed that with the onset of crack tip plasticity, displacements were larger and the stiffness was lower, than in the elastic case. For this reason, he argued that the existing crack behaved as if it were larger than it actually was. Therefore, to account for the behaviour observed, he postulated that an effective crack length, a_{eff} , should be used in the relation for the stress intensity factor, Equation 1.7, thus defining an effective stress intensity value K_{eff} . To accomplish this Irwin used the relations in Table 1.1, for Mode I loading, to define the normal stress, σ_{yy} , to the crack plane ($\theta = 0$) in a linear elastic material as:

$$\sigma_{yy} = K_I / \sqrt{2\pi r} \quad (1.9)$$

A first approximation of the plastic zone size, for plane stress conditions, was given by Equation 1.9 when $\sigma_y = \sigma_{y,s}$:

$$r_y = \frac{1}{2\pi} (K_I / \sigma_{y,s})^2 \quad (1.10)$$

where $\sigma_{y,s}$ is the yield stress. This analysis was not entirely correct since Equation 1.9 was derived for elastic crack tip conditions. The cross hatched area of Figure 1.7 represents the forces that would be present in an elastic material but not an elastic-plastic material because the stress cannot be greater than the yield stress. To account for this discrepancy the plastic zone size was increased by employing a force balance which produced the second estimate of plastic zone size, r_p :

$$r_p = \frac{1}{\pi} (K_I / \sigma_{y,s})^2 = 2r_y \quad (1.11)$$

This estimate was double the original estimate, r_y . Irwin then decided that the best approximations for K_{eff} were attained when the crack tip was placed in the centre of the plastic zone. Thus:

$$a_{eff} = a + r_y \quad (1.12)$$

Under plane strain conditions:

$$r_y = \frac{1}{6\pi} (K_I / \sigma_{y,s})^2 \quad (1.13)$$

which is smaller than the plane stress result since the yielding at the crack tip is suppressed by the triaxial stress state.

Another model which assumes an effective crack which is longer than the physical crack, is the Strip Yield Model, first proposed, independently, by Dugdale [7] and Barenblatt [8]. This model assumed a long slender plastic zone at the crack tip with length ρ , thus making the total crack length $2a + 2\rho$, Figure 1.8(a). In addition a closure stress equal to $\sigma_{y,s}$ was also applied at each crack tip, Figure 1.8(b). The size of ρ is taken such that the stress singularity disappears, resulting in the stress intensity factor being zero. To accomplish this the model approximates the elastic-plastic behaviour as the sum of two elastic solutions: a thru crack under Mode I loading and the same crack with closure stresses at the tip. The addition of the values of K from the two loading situations should cancel each other out to maintain the above assumption. Firstly, the stress intensity factor due to the closure stress is estimated as:

$$K_{closure} = 2\sigma_{y,s} \sqrt{\frac{a+\rho}{\pi}} \cos^{-1} \left(\frac{a}{a+\rho} \right) \quad (1.14)$$

The stress intensity factor of a thru crack under Mode I loading in an infinite plate with $a = a + \rho$ is:

$$K_I = \sigma \sqrt{\pi(a + \rho)} \quad (1.15)$$

Since $K_{closure} + K_I = 0$ the resulting plastic zone size is given by:

$$\frac{a}{a + \rho} = \cos\left(\frac{\pi\sigma}{2\sigma_{y.s.}}\right) \quad (1.16)$$

and the effective stress intensity factor, with $a_{eff} = a + \rho$ is:

$$K_{eff} = \sigma \sqrt{\pi a \sec\left(\frac{\pi\sigma}{2\sigma_{y.s.}}\right)} \quad (1.17)$$

However, this result tends to overestimate K_{eff} , since the actual a_{eff} is slightly smaller than $a + \rho$ because the strip yield zone is loaded to $\sigma_{y.s.}$. For this reason Burdekin and Stone [9] obtained a better approximation of K_{eff} for the strip yield model:

$$K_{eff} = \sigma_{y.s.} \sqrt{\pi a} \sqrt{\frac{8}{\pi^2} \ln \sec\left(\frac{\pi\sigma}{2\sigma_{y.s.}}\right)} \quad (1.18)$$

Equation 1.7 proposed by Griffith is valid only for ideally brittle solids. During his investigations Griffith obtained good agreement between Equation

1.7 and experimental fracture strength of glass, but this theory greatly underestimates the fracture strength of metals. For this reason Irwin [4] and Orowan [5], working separately, modified the Griffith equation to account for plasticity. The revised equation for K is:

$$K = \sqrt{2E(\gamma_s + \gamma_p)} \quad (1.19)$$

where γ_p is the plastic work per unit area of surface created. Typically $\gamma_p \gg \gamma_s$. This term was required because unlike in ideally brittle solids, where a crack can be formed by merely breaking atomic bonds, cracks propagating in metals are accompanied by dislocation motion in the vicinity of the crack tip, which results in an additional energy dissipation. Equation 1.19, although originally derived for metals, can easily be extended to account for any type of energy dissipation:

$$K = \sqrt{2Ew_f} \quad (1.20)$$

where w_f is the fracture energy, which could include plastic, viscoelastic or viscoplastic effects, depending on the material. However, when using Equation 1.20, caution should be exercised for two reasons: (1) The Griffith model applies only to linear elastic material behaviour. Although the behaviour at the crack tip may not be linear the global behaviour of the

structure must be elastic and (2) The value of w_f may not be a constant. In ductile materials the fracture energy varies with time.

To this point the models presented have been LEFM extensions that account for elastic-plastic behaviour. The models produce reasonable results provided the plastic zone size remains small compared with the crack size. This situation occurs when the stress is low with respect to the yield stress. If conditions other than this prevail, then the plastic zone expands beyond the point at which the behaviour can uniquely be expressed in terms of K . For this reason the Crack Opening Displacement and J-integral models have been developed.

The Crack Opening Displacement model introduced by Wells assumes that crack extensions occur when the material at the crack tip reaches some maximum strain level. These strains can be related to the crack opening displacement criteria, which is a measurable quantity. When the crack opening displacement reaches a critical value, failure is assumed to occur. The major drawback of the COD criterion is that there is no direct calculation of the fracture stresses. Therefore, it is primarily a comparative toughness parameter.

In the J-integral method, the crack tip stress field can be expressed for certain idealized elastic-plastic material behaviour as:

$$\sigma_{ij} = C \left(\frac{J}{r} \right)^{1/(n+1)} \xi_{ij}(\theta) \quad (1.21)$$

where n is the strain hardening exponent and J is the J-integral which is similar to K but provides a means for analyzing more extensive plastic behaviour.

1.3 Evolving Microstructure Models

The preceding sections have dealt mainly with the analysis of when i.e. at what critical stress or crack size, a material will fracture. However, no mention was made of how this fracture actually occurs; that is, the mechanisms of fracture. For the most part, the mechanisms involved greatly influence the behaviour observed. This is due to the fact that, as a material is loaded and nonlinearities are introduced, the overall structure of the material also evolves. For example, from a microscopic point of view most structural materials fail by a mechanism known as microvoid coalescence, which results in a dimpled appearance on the fracture surface. This dimpled shape is strongly influenced by the type of load applied, see Figure 1.9. The microvoids which form these dimples nucleate at various internal discontinuities, the most common being intermetallic particles and precipitates, as well as grain boundaries. As the local stress in the now porous material increases these microvoids grow, coalesce and eventually form a continuous fracture surface. A schematic of the initiation, growth and coalescence of these voids can be

seen in Figure 1.10. This figure illustrates the interesting point that the voids can initiate at matrix/particle interfaces as well as by particle fracture. Consequently, it can be concluded that small voids are nucleated by small particles and large voids by large particles. The mechanisms of nucleation, growth and coalescence along with the complexities introduced by void size, shape and interactions limit the effectiveness of LEFM as a tool for modeling overall constitutive behaviour of “porous” materials. As a result, many investigators have concentrated their efforts to produce models for ductile material, which account for one or more of these mechanisms. The remainder of this section will address some of this work.

As a starting point, to account for the aforementioned mechanisms characterizing ductile fracture, researchers began to analyze the growth of single voids. Among the first was McClintock [12] who considered, analytically, the growth of long cylindrical voids with circular and elliptical cross-sections, Figure 1.11, in non hardening material. McClintock restricted the loading to elongation in the direction of the cylindrical axis coupled with applied transverse tensile stresses. As a result, only principal values were considered and no rotations were introduced. In addition, he assumed that, since the voids being considered would remain relatively small throughout the loading history, the components of applied stress and strain could be represented by the stress-strain relations for an incompressible, fully plastic material. A secondary effect of the small void assumption was that void

interactions could be neglected. His investigation yielded estimates for critical strains at void coalescence.

Following McClintock's results, Rice & Tracy [13] obtained critical strain solutions for a more realistic void shape, i.e. an isolated spherical void in a remotely uniform stress and strain-rate field. To accomplish this, Rice & Tracy derived a variational principle governing the void expansion in a rigid-plastic medium and employed a Rayleigh-Ritz procedure for the approximate solution. However, this model, as was the case with McClintock's, does not account for the interaction between neighbouring voids. As a result, these so called finite shell models, produced valid results only when the porosity value was taken to be very small i.e. in the dilute limit. To alleviate this shortcoming, some investigators turned to analyzing the growth of voids in material models which assume a periodic microstructure.

Needleman [23] analyzed numerically the overall deformation of a medium containing a doubly periodic square array of circular voids, Figure 1.12(a). This assumed symmetry allowed the void interaction effects to be accounted for rigorously. In addition, the problem of the entire array was reduced down to a boundary value problem of a single unit cell, Figure 1.12(b). The symmetry of the cell itself was also taken into consideration and only the upper quadrant (EBFC) was modeled numerically by the finite element method. The numerical solution assumed plain-strain deformation perpendicular to the cylinder's axis and straight lines, bounding cells and connecting void centres, would remain straight as the deformation

progressed. The resulting loading versus strain plots, compared with the same for material without voids, can be seen in Figure 1.13(a). The presence of voids lowers the load required to achieve a given strain and decreases the value of strain, U/L_0 , at which the maximum load occurs.

The evolution of the cell can be seen in Figure 1.13(b), which depicts the initiation and growth of a plastic zone, the shaded area, and the change in the void itself, as strain increases. The void is seen to initially elongate in the direction of loading and contract in the transverse direction. As the maximum load is attained contraction in the transverse direction changes to elongation. The plastic zone is seen to begin near the void in on the x^1 axis, followed by a diagonal band which eventually links with the initially observed zone. The plastic zone then continues to grow until it encompasses the whole quadrant, except for a small region above the void. Unloading is seen to begin in the upper corner of the quadrant as the region between the voids necks down rapidly. This model produced more reliable results, than previously attained, because it accounted rigorously for the interaction between neighbouring voids. However, because of the symmetry assumptions made, all voids present in the material deformed in the same manner which was not a realistic situation.

Abeyaratne & Triantafyllidis [24] proposed an alternative representation. A periodic microstructure was still assumed but different voids were allowed to deform differently. To accomplish this representation Abeyaratne & Triantafyllidis assumed a cylindrical block of material whose

cross-section in the undeformed state was a rectangle containing a periodic array of voids with an elliptical cross-section, Figure 1.14(a). The voids in this material were assumed to be spaced $2\epsilon a_1$ (and $2\epsilon a_2$) apart in the x_1 (and x_2) directions, and the semi-major and semi-minor axis of each ellipse were ϵb_1 and ϵb_2 , respectively, Figure 1.14(b). The material around each void was discretized as in Figure 1.14(c) and the symmetry of the block was used to simplify the FEM model to only the upper-right quadrant. The lateral boundaries of the block were assumed to be free of shear tractions and were subjected to prescribed stretches. The numerical results of this representation were then used in a homogenization procedure to portray the material as a whole. It is not hard to see that this type of procedure, while producing accurate results, can become numerically intensive if a more complicated microstructural arrangement were assumed i.e. a three dimensional void.

The next step in models accounting for microstructure was to prescribe bounds for the effective properties of appropriate classes of composites with random microstructures and to account for microstructural changes through the use of evolution equations for variables such as void fraction. Probably the best known porous ductile material model, which implements such an approach, was developed by Gurson [14] who made use of the results of pioneering investigators [12, 13] to produce estimates for the effective properties of rigid perfectly-plastic porous materials, with cylindrical and spherical voids, which accounted for the effects of void growth and nucleation. Due to its popularity, many investigators have subsequently used

Gurson's model, with slight modifications, to account for various phenomenon, i.e. void interactions (Tvergaard [15]), void coalescence (Tvergaard & Needleman [16]) and void shape effects (Becker et al [17]).

In the spirit of Gurson, Duva & Hutchinson [18] applied earlier results of Budiansky et al [19], for spherical voids in unbounded nonlinearly viscous solids, to obtain estimates of the effective behaviour of porous nonlinearly viscous materials with dilute concentrations of spherical voids. As an extension to this model, Lee & Mear [20] obtained solutions for spheroidal void shapes under the special case of axisymmetric loading conditions (aligned with the principal axes of the voids). Simplified models have arisen from these results, for perfectly plastic materials with aligned spheroidal voids subjected to axisymmetric loading conditions, due to the work of Golaganu et al [21] and [22].

Ponte Castaneda & Willis [25] applied the effective property method to nonlinearly viscous materials. Their efforts produced bounds for the effective potentials, of porous and rigidly reinforced materials with isotropic microstructures. They achieved this by applying a nonlinear extension of the Hashin-Shtrikman [26] variational principles. This approach was first introduced by Willis [27] and further developed by Talbot & Willis [28]. Willis & Talbot [29] generalized these bounds to materials with special classes of anisotropic microstructures.

Recently, Ponte Castaneda [30] used a different method, based on variational principles, to produce improved Hashin-Shtrikman bounds for

isotropic microstructures. These improved bounds for the effective potentials, were derived alternatively by Willis [31] and Suquet [32]. Alternatively, results for special classes of anisotropic composites have been developed by Talbot & Willis [33], Ponte Castaneda and DeBotton [34] and Suquet [32].

The constitutive model used in the present work was developed by Ponte Castaneda & Zaidman [35] and will be referred to as the PCZ model. It makes use of the results for porous materials with a special class of anisotropic microstructures, introduced by Talbot & Willis [33]. The explicit results are computed for the anisotropic yield surfaces of rigid perfectly-plastic composites with aligned ellipsoidal voids.

Most of the models mentioned above produce adequate results [35] when the deformations are assumed to be small, thus assuring that the microstructure remains essentially fixed. However, with larger deformations the microstructures may change in any of the following ways: (1) size, (2) shape, (3) orientation of voids or (4) positioning of the voids with respect to each other. These changes, or put another way the “evolution” of the microstructure, affects the effective response of the porous material. To be able to account precisely for these effects it is necessary to solve the exact (nonlinear) boundary value problem for the local fields within the porous material. This is a daunting task indeed if one considers the complexity of actual microstructures. However, solutions for highly idealized microstructures have been attained, recall Abeyaratne & Triantafyllidis [24]. The PCZ model applies such a simplified scheme by identifying appropriate

“internal variables” which characterize the “state” of the microstructure. These “state variables” are updated with the evolution equations. These evolution equations for porosity (size) and variables characterizing shape of the voids (aspect ratio) are used in conjunction with the constitutive relations for the nonlinear anisotropic porous composites to define the overall behaviour. This is done under the assumption of triaxial loading conditions, aligned with the material symmetry axis of the composites, so that these axes do not rotate as the deformation progresses. The rotation of the material axis may also be taken into account but introduces complications which were not pursued in this model.

Although the effects of the evolution of state variables have not been considered explicitly in the development of large deformation constitutive models for porous materials, the behaviour of isolated voids dispersed in unbounded media, as was presented earlier, has been studied by several authors. Eshelby [36], found that the strain field within an ellipsoidal inclusion, embedded in an unbounded linear-elastic solid, is constant if the surrounding material is subjected to uniform stress or strain conditions on its boundary. Budiansky et al [19] and Fleck & Hutchinson [37] noted the mathematical analogy between the equations of linear-elasticity and Stokes’ equations for slow flow in a viscous fluid and interpreted Eshelby’s results to imply that ellipsoidal voids in a linearly viscous fluid, subjected to a uniform boundary condition, will remain ellipsoidal but vary in size, shape and orientation. They used this observation to study the evolution of initially

spherical voids in linearly viscous fluids under axisymmetric and combined hydrostatic-shear loading respectively. In addition, the same authors also studied the growth rates and changes in aspect ratio of specific void shapes in nonlinearly viscous materials, proving that Eshelby's results also appear to hold approximately in nonlinear viscous materials.

Although the contribution of these authors greatly advanced research in this area of study, the PCZ model goes beyond their results and includes the effects of microstructural evolution into an approximate constitutive model for nonlinear porous material. Accounting for these effects has significant implications to the effective behaviour of the porous materials. One such effect is the difference in behaviour between porous materials undergoing finite deformations and that observed for the matrix material from which they are made. For example, porous materials with perfectly-plastic matrices are not themselves perfectly-plastic i.e. they may exhibit hardening or even softening depending on the specific loading conditions. This phenomenon also was predicted by the model of Gurson [14], with an evolution law for porosity, however the evolution of pore shape, which was not accounted for by Gurson's model because the voids were assumed to remain spherical, produces greatly different results.

1.4 Present Work

The main goal of the present work is to (1) implement the PCZ model as a constitutive relation in an object oriented code being developed by the Manufacturing Research Corporation of Ontario (MRCO) at Carleton University and (2) analyze the behaviour of this model under different conditions, assessing its validity as a tool for predicting the behaviour of porous material. If acceptable, this application of the PCZ model would aid in the simulation of manufacturing processes, by predicting the effects on the stress-strain relation caused by the evolving size and shape of the voids present in the material being investigated.

Examples of possible applications are: HIPing and forging, as well as structural analysis of castings which may contain voids due to solidification shrinkage. An even more obvious situation where the PCZ model could be used is that of materials which are porous by nature, specifically foams and plastic "honeycomb" materials. From a metals standpoint an ideal situation would be slow deformation with significant populations of voids, such as is seen during secondary creep at elevated temperatures. In general, the PCZ model would be a useful tool in any application where significant plasticity is observed in the presence of voids.

The remainder of this thesis is organized as follows. Chapter 2 outlines the basics behind the PCZ model itself, stating assumptions and presenting a derivation of the major aspects of the model. The emphasis then shifts to the

actual work conducted by the author. In Chapter 3, the simplification of the PCZ model for two specific void types, namely, spherical and spheroidal voids, is presented along with C++ code implementing these simplified constitutive relations. Chapter 4 outlines the testing schedule conducted and tabulates the results of these tests. Finally, Chapter 5 contains some concluding remarks and suggestions for possible future work.

Chapter 2

2.0 The PCZ Constitutive Model

In the following section, the methodology behind the development of the PCZ constitutive model will be presented in detail. To begin, the effective properties will be defined, firstly by standard variational characterizations and then by improved characterization for nonlinear composites suggested by Ponte Castaneda [30, 38]. Subsequently there will be a need to produce estimates for the effective viscosity tensor for porous material. This will again be done by two means: Hashin-Shtrikman estimates and Dilute estimates. Arguments, proposed by Ponte Castaneda & Zaidman [35], as to which is more appropriate will then be outlined. Finally, the resulting evolution and constitutive relations will be defined.

2.1 Effective Properties

The heterogeneous material considered here is referred to as a composite with two distinct phases: the matrix and the heterogeneity, i.e.

void, where the latter is much smaller than the former. It should be noted that the effective properties are in fact the relations between the averages of the local stress and strain (strain-rate) fields within the composite. The standard variational characterizations assumes that the effective properties can be obtained in terms of the energy function for the composite as shown below.

The local constitutive behaviour of the material is given by:

$$D = \frac{\delta U}{\delta \sigma}(x, \sigma) \quad (2.1)$$

where; σ - Cauchy stress

D - Eulerian strain-rate at point x in the composite

U - stress potential that is convex

If the composite is assumed to occupy the domain Ω of unit volume with boundary $\partial\Omega$, then the effective stress-strain-rate relation [39], follows as:

$$\bar{D} = \frac{\delta \bar{U}}{\delta \bar{\sigma}}(x, \bar{\sigma}) \quad (2.2)$$

where; $\bar{\sigma}$ - average stress (over Ω)

$\bar{D}$ - average strain-rate (over Ω)

$\tilde{U}$ - effective stress potential of the composite

The effective potential of the composite can, through the minimum complementary energy principle, be defined as:

$$\tilde{U}(\bar{\sigma}) = \min_{v \in S(\bar{\sigma})} \int_{\Omega} U(x, \sigma) dv \quad (2.3)$$

where;

$$S(\bar{\sigma}) = \{ \sigma | \nabla \cdot \sigma = 0 \text{ in } \Omega \text{ and } \sigma n = \bar{\sigma} n \text{ on } \partial\Omega \} \quad (2.4)$$

is a set of conditions that produces a uniform stress on the boundary. These conditions also insure the presence of a local velocity field v that is related to the strain rate via $D_v = (v_{i,j} + v_{j,i})/2$. The strain rate is in turn related to σ by Equation 2.1, minimizing the energy functional in Equation 2.3. It should also be noted that an implicit assumption that v is small results in the safe omission of any inertia terms.

It was shown by Suquet [40] that for extreme nonlinear behaviour, the governing equations may be identified with Prandtl-Reuss equations for rigid perfectly-plastic solids and the effective potential may be described in terms of an effective yield domain $\tilde{P}$, such that:

$$\begin{aligned}\tilde{U}(\bar{\sigma}) &= \begin{cases} 0 & \text{if } \bar{\sigma} \in \bar{P} \\ \infty & \text{otherwise} \end{cases} \end{aligned} \quad (2.5)$$

The boundary of $\bar{P}$ defines an effective yield function, $\tilde{\Phi}(\bar{\sigma})$, in terms of which [41, 14]:

$$\bar{D} = \dot{\lambda} \frac{\partial \tilde{\Phi}}{\partial \bar{\sigma}}(\bar{\sigma}) \quad (2.6)$$

where $\dot{\lambda}$, is non-negative and is determined from the consistency condition. $\dot{\tilde{\Phi}} = 0$, where the over-dot denotes a total time derivative and therefore depends on the evolution of the microstructure with time.

It should be noted that the standard homogenization procedure implied by Equations 2.2-2.4 assumes that the microstructure remains fixed. In reality, as the material is deformed, the microstructure evolves with time and as a consequence the procedure described by Equations 2.2-2.4 must be applied sequentially as time progresses. This leads to difficulties, except in rather specific cases such as dilute dispersion of ellipsoidal voids [19], since the microstructural evolution depends on the local fields which are not fully determined by the standard homogenization procedures.

For the case of interest here, i.e. nonlinear composites, Ponte Castaneda [30, 38] proposed an alternative variational representation of the effective potential function in Equation 2.3. This representation will allow the effective

potential function of the nonlinear composite to be estimated in terms of estimates for the effective potential functions of linear composites with identical microstructures. For a given 2-phase composite that is made up of nonlinear isotropic phases 1 and 2, with volume fractions $c^{(1)}$ and $c^{(2)}$ such that $c^{(1)} + c^{(2)} = 1$ and with stress potentials $U^{(1)}(\sigma)$ and $U^{(2)}(\sigma)$ respectively, the variational principle gives the following lower bound (or estimate) for U [30, 38]:

$$\tilde{U}(\bar{\sigma}) \geq \max_{\mu^{(r)}, \kappa^{(r)} \geq 0, r=1,2} \left\{ \frac{1}{2} \bar{\sigma} \cdot (\tilde{L}^{-1} \bar{\sigma}) - \sum_{r=1}^2 c^{(r)} V^{(r)}(\mu^{(r)}, \kappa^{(r)}) \right\} \quad (2.7)$$

where;

- μ -shear Modulus
- κ -bulk Modulus
- $\tilde{L}$ - upper bound for the effective viscosity tensor of the class of linear composites with the same microstructure as the given class of nonlinear composites.

and the functions $V^{(r)}(r = 1,2)$ are from an optimization problem:

$$V^{(r)}(\mu^{(r)}, \kappa^{(r)}) = \max_{\sigma} \left\{ \frac{1}{6\mu^{(r)}} \sigma_r^2 + \frac{1}{2\kappa^{(r)}} \sigma_m^2 - U^{(r)}(\sigma) \right\} \quad (2.8)$$

where; $\sigma_m = (\text{tr}\sigma)/3$: hydrostatic stress

$$\sigma_e = \sqrt{(3/2)\sigma' \cdot \sigma'} \quad : \text{equivalent stress in terms of the deviatoric stress } \sigma'$$

As a result of this procedure, an estimate of the effective potential of a nonlinear composite can be obtained. This estimate is conditional on possession of information pertaining to: the volume fractions and a linear bound for the effective viscosity tensor, for a linear composite with similar microstructure. It now remains to present a method for determining the effective viscosity tensor, $\tilde{L}$, for the linear composite.

2.2 Estimates for Linearly Viscous Composites

2.2.1 Hashin-Shtrikman Estimates

This subsection will present estimates for the effective viscosity tensor for 2-phase composites with aligned ellipsoidal inclusions, Figure 2.1. From the figure it can be seen that the inclusions and the distribution of their centres are assumed to have identical "aspect ratios" i.e. $l_i/l_j = L_i/L_j$. Where l_i and L_i refer to the void semi-axis lengths and intervold spacings respectively. The inclusions are associated with phase-2 having viscosity tensor, $L^{(2)}$, and

proportion, $c^{(2)}$. Similarly the matrix phase is phase-1 with $L^{(0)}$ and $c^{(0)}$ representing the viscosity tensor and proportion respectively. To facilitate latter simplifications, i.e. phase-2 will be identified with the void phase, it is assumed $L^{(1)} > L^{(2)}$. In addition to the effective viscosity tensor, the estimates for the average strain-rates in the two phases will also be presented.

Willis [31] demonstrated that the Hashin-Shtrikman variational principles are given in terms of polarization fields relative to a homogeneous comparison material, with viscosity tensor $L^{(0)}$. Subsequently, the estimates for the effective potential of the composite are attained from the different constant polarization fields within each phase. The resultant optimized polarizations can be used to estimate the average strain-rate fields in each phase of the composite. The average strain-rate in phase r is expressed in terms of the strain-intensity tensor $A^{(r)}$ ($r = 1, 2$) and the average strain rate, $\bar{D}$, of the composite such that $D^{(r)} = A^{(r)}\bar{D}$ [42]. The estimates of $A^{(r)}$ from the Hashin-Shtrikman procedure are given by:

$$A^{(r)} = \hat{A}^{(r)} \left(\sum_{s=1}^2 c^{(s)} \hat{A}^{(s)} \right)^{-1} \quad (2.9)$$

where;

$$\hat{A}^{(r)} = \left[I + P^{(0)} \left(L^{(r)} - L^{(0)} \right) \right]^{-1} \quad (2.10)$$

is the strain-intensity tensor associated with a single ellipsoidal inclusion of material $L^{(r)}$ embedded in a matrix of material $L^{(0)}$, subjected to uniform strain-rate $\bar{D}$ on its boundary [36]. The tensor $P^{(0)}$ depends on (1) the properties of $L^{(0)}$ and (2) the shape of the ellipsoidal inclusion. It may be expressed in terms of Eshelby's tensor $S^{(0)}$ (see Appendix A for definition of Eshelby's Tensor):

$$P^{(0)} = S^{(0)}(L^{(0)})^{-1} \quad (2.11)$$

With these expressions for the strain-intensity tensor of a general two phase composite the corresponding Hashin-Shtrikman estimates for the effective viscosity tensor is:

$$\tilde{L} = \sum_{r=1}^2 c^{(r)} L^{(r)} A^{(r)} \quad (2.12)$$

Willis [44] showed that, for the class of composites with random microstructures exhibiting "ellipsoidal" symmetry, this expression gives an upper bound for $\tilde{L}$ when $L^{(0)} = L^{(1)}$ and a lower bound for $\tilde{L}$ when $L^{(0)} = L^{(2)}$. This implies that although this model restricts its attention to the class with identical "aspect ratios", it is possible that the resulting model may also apply for more general classes of "ellipsoidal" microstructure.

2.2.2 Dilute Estimates

If the value of $L^{(0)}$ is identified with the value for $L^{(1)}$ in the above estimates for $A^{(r)}$ and $\tilde{L}$ and a asymptotic expansion for small concentrations of inclusions ($c^2 \ll 1$) is considered the results are:

$$A^{(1)} = \hat{A}^{(1)} + O(c^{(2)}) = I + O(c^{(2)}) \quad (2.13a)$$

$$A^{(2)} = \hat{A}^{(2)} + O(c^{(2)}) = [I + P^{(1)}(L^{(2)} - L^{(1)})] + O(c^{(2)}) \quad (2.13b)$$

and

$$\tilde{L} = L^{(1)} + c^{(2)} \left[(L^{(2)} - L^{(1)})^{-1} + P^{(1)} \right]^{-1} + O(c^{(2)})^2 \quad (2.14)$$

These results are the same as those given by Eshelby [36] for material with dilute concentrations of aligned ellipsoidal inclusions (phase-2) dispersed in a matrix of phase-1. It should be noted that they are exact to the order of 0 and 1 in $c^{(2)}$ respectively. Another feature of these estimates is the fact that, unlike the Hashin-Shtrikman estimates that include interactions between inclusions¹, these estimates are independent of the two point correlation

¹ These interactions appear in the second order terms in $c^{(2)}$, see Willis [43].

function and hence depend only on the size, shape and orientation, and not the position with respect to each other, of the inclusions.

This leaves us with two methods for determining the strain-rate intensity and the effective viscosity tensor. The following section will outline the reasoning behind choosing one over the other, as given by Ponte Castaneda & Zaidman [35], by examining the effect of an evolving microstructure.

2.2.3 Evolution of the Microstructure

The microstructure of the composite may change through essentially two different mechanisms: positions of the inclusions relative to one another may vary, and the size, shape and orientation of the inclusion may also change. As might be expected, prediction of the evolution of the microstructure is an extremely complicated endeavor, unless some simplifying assumptions are made. Two such assumptions, made by Ponte Castaneda & Zaidman [35], are now presented.

Firstly, it is assumed that the principal axis of the applied loading tensor coincides with the material's symmetry axis i.e. the ellipsoidal inclusion's axis and the loading axis coincide. This will insure that the inclusions do not change orientation as loading progresses. It also must be noted that, for higher fractions of inclusions, individual inclusions may

change orientation but the overall symmetry axes of the composite will remain fixed.

Secondly, the volume fractions of inclusions will be taken to be small but not necessarily infinitesimal. The reasoning being that in the dilute estimate it was observed that only the size, shape and orientation of the inclusions effect the effective properties of the composite. Also, for dilute composites, the estimates for strain-rate intensity can be used to calculate exactly the evolution of size and shape of the inclusion, while maintaining that ellipsoidal inclusions will remain ellipsoidal for general uniform loading conditions [36]. However, the Hashin-Shtrikman estimates can be applied at arbitrary values of inclusion volume fraction but are limited by their dependence on the spacing between inclusions. Also, these estimates assume “ellipsoidal” symmetries (i.e. $l_1/l_3 = L_1/L_3$) for the composites, where in actual fact, due to differences in strain-rate, the spacing and size of the inclusions will change in different proportions, thus destroying the symmetry in the above defined sense.

All these problems point to the Hashin-Shtrikman estimates being too restrictive to account for the evolution of the microstructure precisely. Regardless, these estimates are exact in the dilute limit and coupling this with the knowledge that the contribution of the distribution of the inclusions is only of order two in the volume fraction of the inclusions, give some merit to employing the Hashin-Shtrikman estimates in the evolving microstructure problem, even at small but non dilute concentrations of

inclusions. This is expected to be especially true when the inclusion phase is assumed more compliant than the matrix phase, as was done here, so that deformations are concentrated at the inclusions.

As a result, the PCZ model employs the Hashin-Shtrikman estimates, Equation 2.9, for porous material with “ellipsoidal” symmetry to estimate the evolution of the microstructure under general triaxial loading conditions aligned with the porous materials symmetry axis. These resulting estimates are then be used in Equation 2.12 to generate a value for the effective viscosity tensor of the linearly viscous porous materials with evolving microstructure.

The following section will now combine the results of the previous sections to define the overall constitutive model, as presented by Ponte Castaneda & Zaidman [35], for nonlinearly viscous materials with evolving microstructure.

2.3 The Resulting Model for Nonlinearly Viscous Porous Materials with Evolving Microstructures

First off, the variational representation of the effective potential function for nonlinear composites, Equation 2.7, is specialized to the case where the inclusions are vacuous ($U^{(2)} = 0$) and the matrix phase is incompressible and isotropic with potential $U^{(1)}(\sigma) = \varphi(\sigma_e^2)$ where φ is a

general convex function such that $\varphi(0) = 0$. Then the results of this special case are coupled with the estimates of Hashin-Shtrikman, Equation 2.12, for linear composites with “ellipsoidal” microstructures resulting in, by the same arguments as Ponte Castaneda [30], the following lower bound for the effective potential of the nonlinear composite:

$$\tilde{U}(\bar{\sigma}) \geq (1-f)\varphi\left(\frac{Q^2}{1-f}\right) \quad (2.15)$$

where; $f = c^{(2)}$ = void fraction (porosity)
 Q is defined by the relation:

$$\frac{1}{6\mu^{(1)}}Q^2 = \frac{1}{2}\bar{\sigma} \cdot \left\{ \left[I + \frac{f}{1-f}(I - S^{(1)})^{-1} \right] (L^{(1)})^{-1} \bar{\sigma} \right\} \quad (2.16)$$

This bound was first identified by Ponte Castaneda [30] for isotropic microstructures and then generalized to the class of ellipsoidal microstructures, which are considered here, by Talbot & Willis [33].

Further simplifications are attained if one assumes spheroidal symmetry i.e. $l_1 = l_2$. This class exhibits overall transversely isotropic symmetry and Equation 2.16 can be rewritten as:

$$Q^2 = q_1 \bar{\sigma}_p^2 + \frac{1}{2} q_2 \bar{\sigma}_n^2 + q_3 \bar{\tau}_p^2 + q_4 \bar{\tau}_n^2 + 2q_5 \bar{\sigma}_p \bar{\sigma}_n \quad (2.17)$$

where: $q_1 \rightarrow q_5$ are functions of f and void aspect ratio
aspect ratio = $w = w_1 = w_2$ (see Appendix A)
and $\bar{\sigma}_p$, $\bar{\sigma}_n$, $\bar{\tau}_p$, and $\bar{\tau}_n$ are a set of transversely
isotropic invariants of $\bar{\sigma}$ defined as:

$$\bar{\sigma}_p = \frac{1}{2} (\bar{\sigma}_{11} + \bar{\sigma}_{22}) = \text{in plain hydrostatic tensile stress}$$

$$\bar{\sigma}_n = \bar{\sigma}_{33} = \text{normal tensile stress}$$

$$\bar{\tau}_p = \sqrt{\bar{\sigma}_{12}^2 + \frac{1}{2} (\bar{\sigma}_{11} - \bar{\sigma}_{22})^2} = \text{transverse shear stress}$$

$$\bar{\tau}_n = \sqrt{\bar{\sigma}_{13}^2 + \bar{\sigma}_{23}^2} = \text{longitudinal shear stress}$$

For the special case of spherical voids [30]:

$$Q^2 = \bar{\sigma}_e^2 + \frac{f}{1-f} \left(\frac{2}{3} \bar{\sigma}_e^2 + \frac{9}{4} \bar{\sigma}_m^2 \right) \quad (2.18)$$

It may be noted that in general the potential functions of a nonlinear material will also depend on the determinant of the stress, i.e. the cubic invariant, [35] however the above estimation neglects this dependence.

For the special case of a rigid perfectly-plastic matrix material the effective behaviour of the porous composite is expressed in terms of the effective yield function, defined in Equation 2.5, and given as:

$$\bar{\phi}(\bar{\sigma}) = \frac{[Q(\bar{\sigma}, f, w_1, w_2)]^{\frac{1}{n}}}{(1-f)\sigma_y} - \sigma_y \quad (2.19)$$

where σ_y is the yield stress of the isotropic Mises matrix.

This is in fact a rigorous upper bound for the yield surface of this class of rigid perfectly-plastic porous materials with ellipsoidal symmetry [35]. As a result of Equation 2.19 being employed, the stress-strain-rate relation must be defined by Equation 2.6.

It is noted that these results apply instantaneously for general loading conditions and are known to have certain limitations, Ponte Castaneda [35]. For instance, the potential, Equation 2.15, can be expected to be inaccurate, for isotropic microstructures, when nearly hydrostatic loadings are applied to the composite. The relative error increases with increasing nonlinearity and decreasing porosity. However, it was found to be reasonably accurate for porosities in the order of 10% [35]. Improvement of these bounds are possible, however, the changes in the qualitative behaviour of the results, other than for loading conditions involving a relatively large hydrostatic component, are not likely [35].

Shifting emphasis now to the equations for the evolution of the microstructure, it should first be remembered that loading is restricted to triaxial loading aligned with the material symmetry axis of the porous composite. The evolution law for porosity is well known from the work of Gurson [14] and takes the following form for incompressible behaviour of the matrix:

$$\dot{f} = (1 - f)\bar{D}_u \quad (2.20)$$

On the other hand, the rates of change of the aspect ratio of the voids can be related to the uniform strain-rate, $D^{(2)}$, within the voids via the kinematic relations [35]:

$$\begin{aligned} \dot{w}_1 &= (D_{33}^{(2)} - D_{11}^{(2)})w_1 \\ \dot{w}_2 &= (D_{33}^{(2)} - D_{22}^{(2)})w_2 \end{aligned} \quad (2.21)$$

In the case of linear composites, $D^{(2)}$ can be estimated in terms of the Hashin-Shtrikman estimates for the strain-rate intensity tensor $A^{(2)}$. For nonlinear composites it was proposed that the same estimates be used for $A^{(2)}$ but with the optimized values of $\mu^{(1)}$, $\kappa^{(1)}$ and $\mu^{(2)}$, $\kappa^{(2)}$ resulting from the variational representation, Equation 2.7, of the effective potential of the nonlinear composite. For the special case of porous nonlinear materials with an

incompressible matrix ($\mu^{(2)} = \kappa^{(2)} = 0, \kappa^{(1)} = \infty$) the relevant strain-intensity tensor is [35]:

$$A^{(2)} = [I - c^{(1)} S^{(1)}]^{-1} \quad (2.22)$$

and is independent of $\mu^{(1)}$. Therefore, the resulting evolution equations for the aspect ratios are [35]:

$$\begin{aligned} \dot{w}_1 &= w_1 (A_{33ij}^{(2)} - A_{11ij}^{(2)}) \bar{D}_{ij} \\ \dot{w}_2 &= w_2 (A_{33ij}^{(2)} - A_{22ij}^{(2)}) \bar{D}_{ij} \end{aligned} \quad (2.23)$$

which is precisely the same as the corresponding relations for a linearly viscous porous material. However, this doesn't imply that the evolution will be the same since these equations must be solved in conjunction with the constitutive relations, which are quite different for nonlinear composites [35].

As was stated above, the stress-strain-rate relation will take the form of Equation 2.8. Therefore, the quantity $\dot{\lambda}$ must still be defined for the special case of rigid perfectly-plastic porous composites. As was mentioned in Section 2.1 this term is attained by applying the consistency condition that results in:

$$\dot{\Phi}(\bar{\sigma}, f, w_1, w_2) = \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_{ij}} \dot{\bar{\sigma}}_{ij} + \frac{\delta \bar{\Phi}}{\delta f} \dot{f} + \frac{\delta \bar{\Phi}}{\delta w_1} \dot{w}_1 + \frac{\delta \bar{\Phi}}{\delta w_2} \dot{w}_2 = 0 \quad (2.24)$$

In this relation there is no need to distinguish between the objective Jaumann and Standard time derivative [35] since the special loading conditions assumed here restricts rotation of the principal axes of the applied stress.

Therefore, the final stress-strain-rate relation may be written as:

$$\bar{D}_y = \frac{1}{H} \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_y} \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_u} \bar{\sigma}_u \quad (2.25)$$

where H is the rate of hardening, given by [35]:

$$H = - \left[(1-f) \frac{\delta \bar{\Phi}}{\delta f} \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_u} + \left(w_1 \frac{\delta \bar{\Phi}}{\delta w_1} \right) \left(A_{11y}^{(2)} - A_{11y}^{(2)} \right) \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_y} + \left(w_2 \frac{\delta \bar{\Phi}}{\delta w_2} \right) \left(A_{22y}^{(2)} - A_{22y}^{(2)} \right) \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_y} \right] \quad (2.26)$$

Thus, the complete constitutive description of the nonlinearly viscous porous material is given by Equations (2.25), (2.26) and (2.19) with (2.20) and (2.23). The next Chapter describes the implementation of these relations for two specific void types: spherical and spheroidal. The resulting relations and limitations will be summarized. In addition, the C++ constitutive model class, developed to implement this model, will be presented.

Chapter 3

3.0 Application of the PCZ Model for Spherical and Spheroidal Voids

In order to assess the advantages of using the PCZ model as a constitutive relation for porous material, it was decided that a preliminary examination should focus on investigating the approximations derived for two simplified void shapes: (i) spherical and (ii) spheroidal. To be able to conduct this analysis a program was developed, *PorousMaterial.cc* (Appendix B), that conforms to the style, dictated by the MRCO, for constitutive relations used in their simulation code for manufacturing processes. Although not a stand alone program, *PorousMaterial.cc* is supplied with the ability to interact with the finite element simulation code, that it will eventually be linked with, and acts as a tool for assessing the stress-strain behaviour of porous material.

Recalling, from Chapter 2, the overall PCZ constitutive description is given by the relations for the; Stress-Strain Rate (Equation 2.25), Hardening Rate (Equation 2.26), Effective Yield Function (Equation 2.19), Void Volume Fraction Evolution (Equation 2.20) and the Void Aspect Ratio Evolution (Equation 2.23). The present chapter will outline the simplifications and assumptions, made to these governing equations, accounting for the

restrictions imposed on the void shape. In addition, the implementation of the constitutive relation will be divided into specific calculation steps and their corresponding functions in PorousMaterial.cc will be noted. As well, supplementary functions required by the simulation code, but not directly associated with the PCZ model, will be mentioned.

Before the limitations imposed by the assumed void shape are presented, it should be noted that the above mentioned governing equations were developed under two major assumptions:

- The PCZ model, assumes that (from Section 2.2.3) “the principal axis of the applied loading tensor coincides with the materials symmetry axis i.e. the ellipsoidal inclusion’s axis and the loading axis coincide”. This assumption was made to insure that there was no rotation of the voids during loading and leads to only principal stress and strain values being used in all calculations:

$$\begin{aligned}\bar{\sigma}_y &= 0 \\ \bar{D}_{ij} &= 0 \quad \text{for } i \neq j \\ \dot{\bar{\sigma}}_y &= 0\end{aligned}\tag{3.1}$$

- The PCZ model was developed using a rigid perfectly-plastic assumption for the matrix material i.e. $\nu_{\text{matrix}} = 0.5$, in order to examine the hardening characteristics induced by the voids exclusively.

With these assumptions in mind the simplifications for the assumed void shapes will now be presented.

3.1 Stress-Strain Rate Relation

The stress-strain rate relation is the mapping of the stress rate vector, $\dot{\bar{\sigma}}_u$, onto the strain rate vector, $\bar{D}_y$, and takes the form:

$$\bar{D}_y = \frac{1}{H} \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_y} \frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_u} \dot{\bar{\sigma}}_u \quad (3.2)$$

For the two void shapes under investigation, the differences in this mapping arises from the relations for the effective yield function, $\bar{\Phi}$, and the hardening rate, H . As a result, these two components will now be examined.

The effective yield function is given by:

$$\bar{\Phi}(\bar{\sigma}) = \frac{[Q(\bar{\sigma}, f, w_1, w_2)]^{\frac{1}{n}}}{(1-f)\sigma_y} - \sigma_y \quad (3.3)$$

where the relation Q^2 is defined by Equations 2.17 and 2.18 for spheroidal and spherical voids respectively. The spherical representation can be implemented easily by direct substitution of the stress values and void

volume fraction. However, problems were encountered for the spheroidal case when the aspect ratio, w , approached unity. The cause was traced to the function, h , used in the definition of q_i , $i = 1..5$ (see Equation 2.17 and Appendix A for details). Although Ponte Castaneda and Zaidman [35], stated that these relations were used for $w = 1$, this is highly unlikely since at this value $h = 0$. This translates into a discontinuity in h , Figure 3.1, that would adversely effect the value of the effective yield function. The continuous nature of h that is more desirable, and undoubtedly the intended form, can be seen in Figure 3.2. To attempt to alleviate this apparent shortcoming, a “tolerance zone”, around $w = 1$, was established by examining Figure 3.1. If the aspect ratio falls in the range:

$$1.0 - \varepsilon < w < 1.0 + \varepsilon \quad (3.4)$$

where $\varepsilon = 1.0e-4$, then the calculations, involving h , will be conducted with aspect ratio values of $1.0 - \varepsilon$ or $1.0 + \varepsilon$ depending on which side of unity the actual value falls. Another possibility, that may have been more appropriate, in light of results to be seen later, would be to enforce a linear interpolation function in this zone to maintain the continuity of h . However, the anomaly was addressed as presented and the obtained results reflect this approach. The next step in calculating the stress-strain rate relation is to examine the hardening rate.

The hardening rate, given by the PCZ model, takes the form:

$$H = - \left[(1-f) \frac{\partial \tilde{\Phi}}{\partial f} \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{kk}} + \left(w_1 \frac{\partial \tilde{\Phi}}{\partial w_1} \right) (A_{11ij}^{(2)} - A_{1ij}^{(2)}) \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{ij}} + \left(w_2 \frac{\partial \tilde{\Phi}}{\partial w_2} \right) (A_{22ij}^{(2)} - A_{2ij}^{(2)}) \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{ij}} \right] \quad (3.5)$$

This equation assumes that the voids are general ellipsoids i.e. $w_1 \neq w_2$. For the case of spherical voids, $w_1 = w_2 = w = 1.0$, the hardening rate can be simplified to:

$$H = - \left[(1-f) \frac{\partial \tilde{\Phi}}{\partial f} \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{kk}} \right] \quad (3.6)$$

$$\text{since} \quad \frac{\partial \tilde{\Phi}}{\partial w_1} = \frac{\partial \tilde{\Phi}}{\partial w_2} = 0 \quad (3.7)$$

As for spheroidal, voids $w_1 = w_2 = w = 1.0$, the hardening rate was seen to be:

$$H = - \left[(1-f) \frac{\partial \tilde{\Phi}}{\partial f} \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{kk}} + \frac{1}{2} \left(w \frac{\partial \tilde{\Phi}}{\partial w} \right) (2A_{33ij}^{(2)} - A_{11ij}^{(2)} - A_{22ij}^{(2)}) \frac{\partial \tilde{\Phi}}{\partial \tilde{\sigma}_{ij}} \right] \quad (3.8)$$

This relation is somewhat different from what was first expected when the spheroidal void case was examined. The reasoning for adopting this assumption can be seen in Appendix A and calculations pertaining to the hardening rate are found in the function, `HardeningRate`, of `PorousMaterial.cc`.

All the components of the stress-strain rate relation can be calculated at this point. To facilitate programming of these constituents, Equation 3.2 will

now be represented in matrix form, which is more conducive to being programmed. The general form of the following equations will be the same regardless of void shape, although differences will occur in the components of the individual matrices.

It is assumed that $\frac{\delta\bar{\Phi}}{\delta\bar{\sigma}_y}$ can be represented as:

$$\left\{ \frac{\delta\bar{\Phi}}{\delta\bar{\sigma}} \right\} = [B] \{ \bar{\sigma} \} \quad (3.9)$$

Where:

$$\left\{ \frac{\delta\bar{\Phi}}{\delta\bar{\sigma}} \right\} = \begin{Bmatrix} \frac{\delta\bar{\Phi}}{\delta\bar{\sigma}_{11}} \\ \frac{\delta\bar{\Phi}}{\delta\bar{\sigma}_{22}} \\ \frac{\delta\bar{\Phi}}{\delta\bar{\sigma}_{33}} \\ 0 \\ 0 \\ 0 \end{Bmatrix} \quad (3.10)$$

$$\{\bar{\sigma}\} = \begin{Bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{33} \\ 0 \\ 0 \\ 0 \end{Bmatrix} \quad (3.11)$$

and $[B]$ is a 6x6 mapping matrix whose components can be determined by direct calculation of the derivatives $\frac{\delta \bar{\Phi}}{\delta \bar{\sigma}_i}$ and is formed in the function `B_Matrix` of `PorousMaterial.cc`. As a result, the stress-strain rate relation will take the form:

$$\{\dot{\bar{D}}\} = \frac{1}{H} [B] \{\bar{\sigma}\} \{\bar{\sigma}\}^T [B]^T \{\dot{\bar{\sigma}}\} \quad (3.12)$$

Where the strain and stress rates, $\{\dot{\bar{D}}\}$ and $\{\dot{\bar{\sigma}}\}$ respectively, are represented in the vectorial form similar to that of Equations 3.10 and 3.11. Collecting the stress vector terms into a matrix, Ψ , gives;

$$\{\dot{\bar{D}}\} = \frac{1}{H} [B] \Psi [B]^T \{\dot{\bar{\sigma}}\} \quad (3.13)$$

where, remembering that only the principal values are considered:

$$[\psi] = \begin{bmatrix} \sigma_{11}^2 & \sigma_{11}\sigma_{22} & \sigma_{11}\sigma_{33} & 0 & 0 & 0 \\ \sigma_{11}\sigma_{22} & \sigma_{22}^2 & \sigma_{33}\sigma_{22} & 0 & 0 & 0 \\ \sigma_{11}\sigma_{33} & \sigma_{33}\sigma_{22} & \sigma_{33}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (3.14)$$

Now grouping terms in Equation 3.13:

$$\{\bar{D}\} = [\dot{K}]\{\dot{\sigma}\} \quad (3.15)$$

where $[\dot{K}] = \text{Dynamic Stiffness Matrix} = \frac{1}{H}[B][\psi][B]^T$ and is calculated in PorousMaterial.cc by the function FormDynStiff. To facilitate the linking of PorousMaterial.cc with the manufacturing simulation code, that employs finite element analysis, Equation 3.15 should be put in the form:

$$\{\dot{\sigma}_i\} = [\dot{K}]^{-1}\{\bar{D}_i\} \quad (3.16)$$

However, it was found that $[\dot{K}]$ was rank deficient, possessing a rank of only

1. Although $[B]$ is an invertible matrix, examining $[\psi]$ revealed that $\det_{\psi} = 0$ and thus the result that $[\dot{K}]$ was unable to be inverted. This limits the use of the PCZ model to a rather small number of possible loading conditions involving prescribed values of both stress and strain rates. A possible solution

to this problem is to apply a pseudo-inverse procedure to $\begin{bmatrix} \dot{K} \end{bmatrix}$, thus producing at least an estimate of the behaviour produced by the PCZ model. This procedure will now be outlined.

3.1.1 The Pseudo-Inverse [46]

If there exists a system defined as:

$$Ax = b \quad (3.17)$$

where A - is an $m \times n$ matrix

for every x , Ax is in the column space of A , it is a combination of the columns of A weighted by the components of x . Such a situation can be seen in Equation 3.15, where A , x and b are analogous to $\dot{K}$, $\vec{\sigma}$ and $\overline{D}$ respectively. The optimal solution, $A\bar{x}$, minimizes the error by projecting b onto the column space at point, p , such that:

$$A\bar{x} = p \quad (3.18)$$

When there is only one combination of columns of A that produce p , the weights of this combination define the solution $\bar{x}$. This situation arises when:

- (i) The columns of A are linearly independent.
- (ii) The nullspace of A contains the zero vector.
- (iii) The rank of A is n .
- (iv) The square matrix $A^T A$ is invertable.

and $\bar{x}$ is defined by:

$$\bar{x} = (A^T A)^{-1} A^T b \quad (3.19)$$

Equation 3.19 includes the case when A itself is invertable. In this case $\bar{x}$ will be the one and only solution to the original system, Equation 3.17:

$$\bar{x} = A^{-1} (A^T)^{-1} A^T b = A^{-1} b \quad (3.20)$$

More generally, the pseudo-inverse (Moore-Penrose inverse), A^* , can be defined as a matrix that defines $\bar{x}$, given any coefficient matrix A and any right side b . Included are the cases when A is invertable, in which case $A^* = A^{-1}$, or other cases when the above conditions, (i)-(iv), are met and $A^* = (A^T A)^{-1} A^T$. However, if those same conditions are not satisfied A^* remains to be defined, such is the case in the stress-strain rate relation of

Equation 3.15 since the conditions outlined above are violated. In such a situation, a choice of one of the vectors satisfying Equation 3.18 must be made, such that the optimal solution is the one that has the minimum length i.e. the optimal stress rate vector will be a solution to Equation 3.15 but posses the minimum length of all the possible solutions. In order to make this choice it should be remembered that the nullspace and rowspace of A are orthogonal and as a result any solution may be split in two: the row space component and the null space component. Splitting the optimal solution results in:

$$\bar{x}_o = \bar{x}_r + \bar{x}_n \quad (3.21)$$

where $\bar{x}_o$ - optimal solution
 $\bar{x}_r$ - row space component
 $\bar{x}_n$ -null space component

Given that; (1) $\bar{x}_r$ itself is a solution of Equation 3.18 since $A\bar{x}_n = 0$,
 (2) All solutions include $\bar{x}_r$ (the particular solution) with varying nullspace component (arbitrary solution),
 (3) The length of solutions obey Pythagoras' Law, since the two components are orthogonal,

then the solution with the minimum length is $\bar{x}_r$. Therefore, choosing the nullspace component to be zero, leaves a solution entirely in the row space.

Summarizing, the optimal solution of any system, Equation 3.17, is a vector $\bar{x} = \bar{x}_o$, that is determined by two conditions:

- (a) $A\bar{x}$ equals the projection of b onto the column space of A
- (b) $\bar{x}$ lies in the row space of A .

The matrix that produces this result is the pseudo-inverse, A^+ (K^+ in the case of Equation 3.15):

$$\bar{x} = A^+ b \quad (3.22)$$

One way that this pseudo-inverse may be obtained is by applying a singular value decomposition on the matrix A resulting in:

$$A = U^T \Sigma V \quad (3.23)$$

where

- A - an $m \times n$ matrix
- U - an $m \times m$ orthogonal matrix
- V - an $n \times n$ orthogonal matrix
- Σ - a diagonal matrix with positive numbers in the first r -entries and zero otherwise.

The non-zero diagonal values of Σ correspond to the singular values, u_i , and the number of which correspond to the rank of A . Subsequently, the pseudo-inverse can be defined as:

$$A^* = V^T \Sigma^* U \quad (3.24)$$

where Σ^* is also a diagonal matrix with entries $1/u_i$. This procedure is implemented on $[K]$ in `PorousMaterial.cc` with function `CalcPseudoInverse`. In practice, it is essential to find very small values of u_i , that may arise due to roundoff errors during the decomposition, and set them equal to zero. If this is not done, these values will transform into unwanted large values in Σ^* , that will overwhelm the pseudo-inverse. This reflects the extreme instability of the rank, and of the pseudo-inverse itself. A tolerance, that is used in `CalcPseudoInverse`, is to check u_i against 100 times the smallest real number recognizable by the computer being used, the so called machine epsilon (MACHEPS) of the computer.

This concludes the presentation of the actual stress-strain rate relations used for the spherical and spheroidal void cases. In order to complete the constitutive description, the evolution equations for void volume fraction and aspect ratio will now be considered.

3.2 Evolution Equations

The evolution of void volume fraction, for both spherical and spheroidal voids, results from the direct application of the relation:

$$\dot{f} = (1 - f)\overline{D}_v \quad (3.25)$$

using the strain rates obtained from the stress-strain rate relations outlined above. This is done in the function, `VoidFractionUpdate`, of `PorousMaterial.cc`.

The evolution of the void shape involves the implementation of:

$$\begin{aligned} \dot{w}_1 &= w_1 (A_{33y}^{(1)} - A_{11y}^{(2)}) \overline{D}_y \\ \dot{w}_2 &= w_2 (A_{33y}^{(2)} - A_{22y}^{(2)}) \overline{D}_y \end{aligned} \quad (3.26)$$

and is conducted in the function `AxisUpdate`. This function first redefines the aspect ratio using Equation 3.26, and then, since the void semi-axis lengths are also required for further calculations, makes assumptions to fix the void shape and obtain the corresponding semi-axis lengths. These procedures are now outlined.

It can be assumed that:

$$V_i = \frac{4}{3}\pi a_i b_i c_i \quad (3.27)$$

where V_i - initial volume of a single void

$a_i b_i c_i$ - initial semi-axis lengths

and

$$N_i = \frac{f_i V_r}{V_i} \quad (3.28)$$

where N_i - initial number of voids in the part of interest

f_i - initial void volume fraction

V_r - total volume of the part of interest

Similarly, for the final (end of calculation step) values;

$$V_f = \frac{4}{3} \pi a_f b_f c_f \quad (3.29)$$

$$N_f = \frac{f_f V_r}{V_f} \quad (3.30)$$

Since this model does not support void initiation or coalescence, Equations 3.28 and 3.30 may be equated. Substituting Equations 3.27 and 3.29 into the result yields:

$$\frac{f_i}{a_i b_i c_i} = \frac{f_f}{a_f b_f c_f} \quad (3.31)$$

Introducing the new aspect ratios obtained from Equation 3.5:

$$\begin{aligned} w_{1f} &= \frac{a_f}{b_f} \\ w_{2f} &= \frac{a_f}{c_f} \end{aligned} \quad (3.32)$$

Equation 3.31 may be rewritten as:

$$\frac{f_i}{a_i b_i c_i} = \frac{f_f w_{1f} w_{2f}}{a_f^3} \quad (3.33)$$

which yields;

$$a_f = \sqrt[3]{\frac{f_f a_i b_i c_i w_{1f} w_{2f}}{f_i}} \quad (3.34)$$

$$b_f = \frac{a_f}{w_{1f}} \quad (3.35)$$

$$c_f = \frac{a_f}{w_{2f}} \quad (3.36)$$

For spherical voids the condition, $radius = a_f = b_f = c_f$, must be enforced therefore assuming that the volume of the void will be maintained:

$$\frac{4}{3}\pi a_f b_f c_f = \frac{4}{3}\pi (radius)^3$$

$$radius = \sqrt[3]{a_f b_f c_f} \quad (3.37)$$

For spheroidal voids the condition will be $b_f = c_f = b_{f2}$ and a_f will remain as calculated by Equation 3.34. Again assuming void volume to remain the same:

$$\frac{4}{3}\pi a_f b_f c_f = \frac{4}{3}\pi a_f (b_{f2})^2$$

$$b_{f2} = \sqrt{b_f c_f} \quad (3.38)$$

Although these same relations, for void fraction and aspect ratio evolution, are used when the pseudo-inverse is employed, instead of using $[\dot{K}]$ directly with prescribed values, there were problems encountered. Since in the pseudo-inverse case it is the stress rates being calculated and not the strain rates, that are used in the evolution relations 3.4 and 3.5, updated values of

f and w do not correspond to the form predicted by the PCZ model. This is due to the fact that the prescribed strain rate values do not conform to the style of those expected by the model. To try and remedy this situation it was proposed that the stress rate values predicted using the pseudo-inverse calculations be used with $[\dot{K}]$ to produce strain rate values that conform to the PCZ model and hence produce better approximations of the evolution of the internal variables.

With this assumption the simplifications introduced to the PCZ model, to account for spherical and spheroidal void shapes, and the corresponding sections of PorousMaterial.cc, that implement the constitutive relation, have been presented. For the most part the preceding description has outlined the simplifications made to each component of the constitutive relation but offered little with regards to the actual application of the PCZ model. The following section will do just that by presenting the interactions and flow between the upper level simulation code and PorousMaterial.cc. Also, a presentation of the major calculation steps internal to PorousMaterial.cc will be presented.

3.3 Application of the PCZ Model

During an actual application, the PCZ model will require that the simulation code provide several pieces of information to facilitate its calculations. Among them will be the physical properties of the matrix phase under investigation, including; Young's Modulus, Poisson's ratio and yield stress. In addition, since the analysis will be discretized into time steps, information pertaining to these steps should include; size of the time step and the principle stress vector, void fraction and void semi-axis lengths at the start of the time step. As well the deformation gradient over the time step, transformed to the principle directions, should also be included. In return the model will pass back the values for the stress vector, void fraction and void semi-axis lengths at the end of the time step. In addition a linear approximation of the estimated stress-strain relation, over the time step, will be produced. A summary of this interaction can be found in Figure 3.3.

Once `PorousMaterial.cc` has the required information from the upper level code it can begin the calculations of the PCZ model, a flow chart of the major components involved in doing so can be seen in Figure 3.4. This chart depicts only the major calculation steps involved in `PorousMaterial.cc`. For this reason it does not include a detailed description of the code. For such a description the reader is referred to Appendix B.

Firstly, to be able to apply the constitutive relations derived for the PCZ model, a non zero stress vector must be available at the beginning of the time

step. If this condition is not met then the PCZ model cannot be used over the time step. For this situation, the original void fraction and semi-axis lengths will be returned to the simulation code and the constitutive relation is assumed to be that predicted by the isotropic elasticity tensor. On the other hand, if a non zero stress vector does exist, the next step is to determine the major loading axis. This determination is required since the PCZ model was formulated for the case where the major loading axis corresponds to the 33-direction. Hence, terms involving the strain intensity tensor, $A_{\mu\nu}^{(2)}$, in Equations 3.8 and 3.26, should be modified appropriately when alternate loading conditions exist. PorousMaterial.cc incorporates a flag, MajorAxis, that is intended to control these modifications. The major loading axis is also required in the calculation of the Eshelby Tensor (Appendix A) that is in turn used to calculate $A_{\mu\nu}^{(2)}$ (Equation 2.22). With the strain intensity tensor defined, all the information required to form the stress-strain rate relation, Equation 3.15, is present. Examining the hardening rate for spheroidal voids, Equation 3.8, it is seen that the second group of terms, here on referred to as the aspect ratio component of the hardening rate, involves the term $\frac{\delta\bar{\Phi}}{\delta\bar{\sigma}_y}$ that has been defined in Equation 3.9. As a result, the next logical step is to assemble the matrix $[B]$ that will then be used to calculate the hardening rate. Together $[B]$ and H will next be used to determine the matrix $[\dot{K}]$ thus completing the stress-strain rate relation, Equation 3.15. At this point, depending on the applied loading conditions two possibilities exist.

1. If a combination of stress rates and strain rates have been prescribed the direct solution using $\begin{bmatrix} \dot{\mathbf{K}} \end{bmatrix}$ can be conducted to complete the two vectors.
2. If no stress rate values were assigned then the PseudoInverse of $\begin{bmatrix} \dot{\mathbf{K}} \end{bmatrix}$ will be calculated and used with the strain rate vector, that is obtained using the time step value and the deformation gradient, to produce the stress rate vector.

In the latter situation, as discussed earlier, the obtained stress rate will be used with $\begin{bmatrix} \dot{\mathbf{K}} \end{bmatrix}$ to produce a strain rate vector that will conform to the style required by the PCZ model. With these strain rate vectors, the updated void fraction is calculated from Equation 3.25. This updated void fraction is then required in the evolution of the aspect ratio to determine the semi-axis lengths, Equation 3.34, after the aspect ratio evolution is predicted by Equation 3.26 using the strain rate vector and $A_{\mu}^{(2)}$. At this point, the constitutive model has been completely applied for the time step, and all that remains is to arrange the results into the form required by the upper level code. This involves updating the initial stress vector with the strain rate values obtained for the time step. In addition a linear approximation to the stress-strain relation over the time step is formulated and returned to the simulation code along with the values of updated void fraction, semi-axis lengths and stress.

This section has outlined the major calculation steps involved in the practical application of the PCZ model. For the sake of completeness, the following section will briefly outline functions, contained in `PorousMaterial.cc` but not previously considered, which are not needed, directly, for the constitutive description but are included to satisfy requirements of the upper level code.

3.4 Additional Functions²

3.4.1 ComputeStress

The upper level code will call this function to implement the PCZ constitutive model. In addition to being the entry point to `PorousMaterial.cc`, `ComputeStress`' main task is to control the flow of calculations, in the constitutive relation, by assigning values to flags and calling the various functions previously discussed. Finally, at the end of the time step, after all calculations are completed, `ComputeStress` will return to the calling program the updated values of: stress via `ResultStress`, void volume fraction and void semi-axis lengths via `ResultIntVariables` and a linear approximation to the stress-strain relation predicted via `ResultD`.

² Additional function descriptions to those presented here can be seen in Appendix A.

3.4.2 Linearization

Since it is required that a linear approximation, to the predicted stress-strain relation, be returned to the calling program, this function has been included. At the time this function is called, both the stress vector and strain vector are known, therefore it is considered that the approximate linear mapping between the two will have a similar form as the isotropic elasticity tensor. However, the values for Young's Modulus (E) and Poisson's Ratio (ν) will be different from those of the elastic case. The elastic form gives:

$$\varepsilon_{11} = \frac{\sigma_{11}}{E} - \nu \frac{\sigma_{22}}{E} - \nu \frac{\sigma_{33}}{E} \quad (3.39)$$

$$\varepsilon_{22} = -\nu \frac{\sigma_{11}}{E} + \frac{\sigma_{22}}{E} - \nu \frac{\sigma_{33}}{E} \quad (3.40)$$

$$\varepsilon_{33} = -\nu \frac{\sigma_{11}}{E} - \nu \frac{\sigma_{22}}{E} + \frac{\sigma_{33}}{E} \quad (3.41)$$

Using the values predicted by the PCZ model and solving any two of: 3.39, 3.40 and 3.41, yields different values of E and ν . It was then proposed that these varying values be calculated and an average of them be used as the modified Young's Modulus and Poisson's Ratio. Although this method will not produce an exact linear representation on the time step it will be a better approximation than using the elastic values. In the event that an average value of the terms can not be calculated or if the PCZ model is not used on

the time step, the isotropic elasticity tensor will be used as the linear approximation.

3.4.3 ElasticityTensor

This function will use the passed values of Young's Modulus and Poisson's Ratio to form the isotropic elasticity tensor. It is implemented to represent the linear approximation described above if the PCZ model is not used during the time step.

This now concludes the description of PorousMaterial.cc, which can be found in its entirety in Appendix B. The following chapter outlines the testing schedule and presents results of the investigations undertaken.

Chapter 4

4.0 Results and Discussion

Before embarking on an analysis of the results obtained by PorousMaterial.cc, it is necessary to be sure that these predictions conform to those obtained by Ponte Castaneda and Zaidman [35], Figure 4.1. To facilitate such a comparison PorousMaterial.cc was first tested under both uniaxial tension and compression. Since the direct solution method, i.e. using $\dot{K}$, was to be used the following values were prescribed: $\bar{D}_{33} = \pm 0.01$, $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$, $\frac{|\bar{\sigma}_{33}|}{\sigma_y} = 0.8$, $w_{start} = 1.0$, $f_{start} = 0.15$ and $\nu = 0.5$. The resulting evolution of: void fraction, aspect ratio, stress and hardening rate were plotted as functions of the logarithmic strain in the axial direction. These plots can be seen in Figures 4.2 and 4.3, for the spherical void case and Figures 4.4 and 4.5, for the spheroidal void case. The results conform well to those of Ponte Castaneda and Zaidman. For the spherical case the void fractions are seen to increase and decrease, as expected, under tensile (Figure 4.2) and compressive (Figure 4.3) loading respectively. This behaviour translates into an overall softening of the material ($H < 0$) under tensile loading due to the increased volume fraction of the voids. Conversely, overall hardening is observed with

decreasing void fraction in compression. When the effect of evolving aspect ratio is introduced, the spheroidal void case, the results are modified accordingly. During tensile loading, Figure 4.4, the void fraction is also seen to increase. However, due to the influence of the increasing aspect ratio, this increase is limited to a finite value, $\approx 18.1\%$, as opposed to the steady rise towards 100% that is observed in the spherical void case. This observation, coupled with the fact that increasing aspect ratio results in hardening, under tensile loading [35], leads to the small overall hardening behaviour observed. As for compressive loading, Figure 4.5, both the fraction of voids and aspect ratio predict void collapse at approximately 80% strain, much lower than the spherical case which predicts a void fraction of $\approx 9\%$ at the same strain level. Examining the plot of hardening rate evolution there is observed an initial softening region followed by an increasing hardening zone. This is a result of the fact that decreasing the aspect ratio, in compression, imposes softening behaviour on the material [35], which initially overwhelms the hardening induced by the decreasing void fraction and as a result the initial softening zone is observed. However, as the loading progresses the hardening due to decreasing f becomes increasingly more dominant and the second zone with increasing hardening is produced.

With PorousMaterial.cc producing results comparable to those obtained by Ponte Castaneda and Zaidman, a testing schedule investigating the results, produced by the PCZ model, for varying conditions was implemented. The tests included:

- (1) Effect of varying Poisson's Ratio.
- (2) Effect of varying the initial stress prescribed.
- (3) Effect of varying the initial void size and shape.
- (4) Cyclic loading analysis with varying average strain levels and strain amplitudes.
- (5) Brief examination of results produced by PseudoInverse, which implements the pseudo inverse procedure on the so called dynamic stiffness matrix, $\dot{K}$.

During these tests, with exception of (4) and (5), the loading conditions were similar to those outlined above with the difference being in the values of Poisson's Ratio, initial stress and initial void properties for (1), (2) and (3) respectively. The details of these tests along with the results will now be presented.

4.1 Poisson's Ratio Tests

At this point, the PCZ model assumes a rigid perfectly-plastic matrix material. As a result, all the hardening effects exhibited are directly a result of the presence of the voids. However, if a more realistic material is to be investigated, there will be a need to account for hardening in the matrix phase. This could be done by a secondary constitutive relation and used in conjunction with PorousMaterial.cc to predict the overall behaviour of the

material. This additional model may assume a Poisson's Ratio other than that of the perfectly-plastic case, $\nu = 0.5$. Therefore, these particular tests were performed in order to assess the effect of using Poisson's ratios, for the matrix material, other than that of the perfectly-plastic case.

Before the results of these tests are examined, it should be noted that the Poisson's ratio is only used during the calculations of the Eshelby Tensor in the PCZ model and that the components of this tensor are inversely proportional to ν (see Appendix A). The Eshelby Tensor is subsequently used to calculate the Strain Intensity Tensor, $A_{\mu\nu}^{(2)}$ which is in turn used in the evolution calculations of the aspect ratio and the prediction of the aspect ratio component of the hardening rate. Since, for the spherical void case, the condition that, $w = 1.0$, is imposed and there is no contribution to the hardening rate from the aspect ratio, the choice of Poisson's ratio has no effect on the obtained results. The only parameters which will be effected by ν are the void semi-axis lengths, but, as will latter be seen, these too have no effect on the constitutive relations. However, such is not the case for spheroidal voids. The evolution of void fraction, aspect ratio, stress and hardening rate, under tensile loading can be seen in Figure 4.6. From these plots it can be seen that Poisson's ratio has little effect on values of aspect ratio and void fraction at small strains. This changes as strain increases and the effects become more noticeable. Due to the inverse proportionality of the components of the Eshelby Tensor to ν , there is observed a greater rate of increase in aspect ratio for smaller Poisson's ratio values. This translates to smaller increases in void

fraction and hence smaller finite limits on f , $\approx 17.8\%$ for $\nu = 0.3$ to $\approx 18.1\%$ for $\nu = 0.5$. A more detailed representation of the variation over values of Poisson's ratio can be seen in Figures 4.7 and 4.8 at 50% and 100% strain respectively. Examining the plot for hardening rate it can be seen that throughout the loading zone presented, all values of ν predict hardening behaviour, however the magnitude of the hardening varies with both ν and accumulated strain. Initially, the major contribution to the hardening rate comes from the aspect ratio component and as a result the magnitude of the rate of hardening decreases with increasing values of Poisson's ratio. At larger strain levels, the softening effect of the increasing void fractions becomes the major contributing factor to the overall hardening rate. This transition of the major hardening component, from the aspect ratio to the void fraction component, occurs sooner for smaller values of Poisson's ratio. Hence, the magnitudes of the rate of hardening begin to order themselves with increasing values as Poisson's ratio is increased, which is the reverse of what was initially observed. This trend can be seen in Figure 4.8.

Similar results, but in the reverse order, can be seen under compressive loading, Figure 4.9, 4.10 and 4.11. The influence of Poisson's ratio is again seen in the rate of change of w , where smaller ν values produce faster decreases. As a result void fraction also decreases at a larger rate with smaller Poisson's ratios. As for the rate of hardening, the aspect ratio component is initially the major contributor to the overall rate, however, as previously mentioned, in compression this translates into an initial softening

zone. The magnitude of the hardening rates, as was the case under tensile loading, order themselves with respect to Poisson's ratio. However, here the magnitudes are seen to initially increase with increasing Poisson's ratio and as the loading progresses, a transition to decreasing magnitude with increasing ν is observed. Also, as strain is increased, and the transition to the void fraction component being the major contributor to the total rate occurs, it is the higher values which undergo the change first. This change in the hardening rate components occurs at the same rate as that observed under tensile loading, however since the smaller values of ν tend to predict an increased approach towards void collapse, the transition has little, if any, noticeable effect on the evolution for these values of Poisson's ratio.

4.2 Initial Stress Level Tests

During the investigation, of the effects of the initial prescribed stress level on the results produced by PorousMaterial.cc, the prescribed loadings were again the uniaxial compression and tension cases previously outlined. However, the Poisson's ratio was restricted to 0.5 and the initial stress level,

$\left(\frac{|\bar{\sigma}_{\text{in}}|}{\sigma_{\text{y}}^{\text{initial}}} \right)$, was assigned the values of 0.5, 0.8 and 0.9. The results obtained

were consistent throughout the testing, both in compression and tension, as

well as for the two void shapes: spherical and spheroidal. For this reason only the compressive loading case for spheroidal voids is presented, Figure 4.12.

Examining the results, it is clear that the stress level has no effect on the evolution of void fraction or aspect ratio. The calculations for these evolutions primarily involve the strain rate values, in addition the Strain Intensity Tensor, $A_{\mu\mu}^{(2)}$, is used in the aspect ratio evolution. Since $A_{\mu\mu}^{(2)}$ is not effected by the stress level it will remain the same for all situations being investigated. This leaves only the strain rate values which may be influenced by the stress level prescribed. Under these loading conditions $\bar{D}_{xx}$ is a prescribed value common to all three stress levels. This leaves $\bar{D}_{11}$ and $\bar{D}_{22}$ which are equal due to the symmetry of the spheroidal void assumption. The conclusion must be made that, in order to produce the results seen here, the PCZ model must calculate $\bar{D}_{11} = \bar{D}_{22}$, to posses the same value at all three stress levels. This is what would be expected given that $\bar{D}_{xx}$ is the same and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout. As for the hardening rate, the level of stress is directly proportional to the observed magnitude. The initial softening zone still appears and the transition of major hardening rate components occurs at approximately the same time.

4.3 Initial Void Size and Shape Tests

The initial voids, up to this point in the testing, have been assumed to be spherical, $w = 1.0$. In order to determine the effects, on the PCZ model, of the choice of initial voids it was decided that the uniaxial tests, on spheroidal voids, be repeated this time varying the aspect ratio and initial size of the voids in the material being investigated.

The initial size of the voids, which is determined by the prescribed semi-axis lengths: a, b and c , should have no effect on the results obtained from PorousMaterial.cc since only the dimensionless aspect ratio is used in the constitutive relations. In order to verify this contention the size of the initial voids were varied in several tests. The results showed that the predictions of PorousMaterial.cc are indeed independent of void size, provided that the initial aspect ratios were the same.

Next, the initial aspect ratios were varied such that $w_{start} = 0.25, 0.5, 1.0, 2.0, 4.0$ and the tensile and compressive tests were repeated with values: $\bar{D}_{\lambda} = \pm 0.01$, $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$, $\frac{|\bar{\sigma}_{33}|}{\sigma_y} = 0.8$, $f_{start} = 0.15$ and $\nu = 0.5$. The results of the tensile test, Figure 4.13, show that larger values of w_{start} tended to predict larger rates of increase of aspect ratio. This translated into a similar increased rate for the void fraction and in turn larger values of the finite limit i.e. $\approx 29\%$ for $w_{start} = 4.0$ to $\approx 15.3\%$ for $w_{start} = 0.25$. The hardening rates predicted vary considerably with w_{start} . For smaller values, $w_{start} < 1.0$, there is

depicted an initially softening zone. This is a result of the coupling of the aspect ratio component of the hardening rate, which predicts softening in tension [35] and the additional softening due to increasing void fraction. As strain is increased the softening due to the aspect ratio component decreases considerable until it actually predicts hardening values after w becomes greater than unity. The hardening behaviour from the aspect ratio component becomes dominant since the softening due to f is rather weak because of the decreased finite limits, on void fraction, noted above. For $w_{start} > 1.0$, the aspect ratio component initially produces hardening behaviour due to the large values of w . The magnitude of the hardening observed decreases as strain is increased and the void fraction component becomes more dominant. This results in a hardening zone with decreasing magnitude, over the entire loading period.

The compressive test results can be found in Figure 4.14. The effect of w_{start} on the rate of change of aspect ratio is, as was seen in tension, that larger w_{start} values predict faster decreases. However, the small w_{start} values correspond to materials which are much closer to void collapse, for this reason the void fraction of these cases exhibit a faster decrease towards zero. The hardening rates for $w_{start} < 1.0$ predict softening behaviour as w decreases [35], but due to the proximity to void collapse, this has little effect on the overall hardening rate, because the f component is dominant and predicts hardening behaviour. This dominance is not relinquished as strain increases and larger hardening values are seen until void collapse. For the cases where

$w_{\text{def}} > 1.0$ there is initially exhibited a zone of softening behaviour since larger values of aspect ratio in compression result in softening. As the aspect ratio is decreased, hardening behaviour is contributed by the aspect ratio component. Although the magnitude of the hardening from the aspect ratio component decreases with decreasing w , the magnitude of the hardening resulting from the f component increases. The f component becomes the major contributor to the overall hardening rate, resulting in increasing magnitude of hardening behaviour with strain.

4.4 Cyclic Loading

The previous sections have been devoted to examining the results, predicted by the PCZ model, under uniaxial tension and compression, while various initial conditions were applied. The complex interplay between the void fraction and aspect ratio components of the overall hardening rate were observed. This section will deviate from this and present results of cyclic loading tests with varying prescribed average strain values and amplitudes.

4.4.1 Tensile Zone

4.4.1.1 Varying Prescribed Average Strain Level

The strain level prescribed to the PCZ model was varied by applying different forms of a cyclic strain rate, $\bar{D}_{31}$. These strain rates can be seen in Figure 4.15. They all possess a “preloading” section which is used to accumulate the desired strain level before an oscillatory loading, with fixed amplitude of 0.01, is applied. The three average strain levels investigated are 0.1597, 0.0812 and 0.0340. The accumulated strain produced by these prescribed strain rates is presented in Figure 4.16. In addition, the initial conditions for these tests are as follows: $\frac{|\bar{\sigma}_{31}|}{\sigma_y} = 0.8$, $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout, $w_{spher} = 1.0$, $f_{spher} = 0.15$ and $\nu = 0.5$.

When the spherical void case is investigated these cyclic loading conditions produce unexpected results, Figure 4.17. Throughout the 10 000 loading cycles there is seen a steady decrease in void fraction for all strain levels. In fact the rate of void decrease appears to be the same regardless of the average strain level present. The only difference, between the strain levels, is the value of the void fraction at the beginning of the cycling, which is determined by the preloading applied. As for the hardening rate, it initially predicts the softening behaviour resulting from the preloading but as cycles accumulate the softening behaviour gives way to the hardening associated

with the decreasing void fraction. The result is a steady decrease in the softening behaviour.

In the spheroidal void case, Figure 4.18, the preloading section predicts results which are expected i.e. the larger the average strain then the larger the void fraction and aspect ratio. As cyclic loading is introduced, interesting results are predicted. As would be expected under tensile loading the void fraction is seen to increase. The rate of increase of void fraction at higher average strain levels is seen to be lower, which is due primarily to the larger aspect ratios present in these conditions. The interesting results are seen with regards to the aspect ratios. With increasing number of cycles, the PCZ model predicts decreasing aspect ratios. This observation reveals that the loading produces no void growth in the primary loading direction but growth occurs instead in the minor directions, much like crack growth. The hardening rate reflects these results but predicts an initial zone of hardening due to the preloading. The magnitude of the hardening behaviour then rapidly decreases until increased softening behaviour is observed due to the onset of void collapse. Perhaps, in this case, void collapse is not an appropriate term since the void fraction is increasing instead of the decreasing toward zero usually associated with void collapse. Instead this may be predicting void coalescence.

In addition, there may be noticed small deviations in the otherwise smooth curves representing the change in aspect ratio and stress occurring when the aspect ratio passes through the value $w = 1.0$. These, may be directly

attributed to the approximations, discussed previously, to the calculations at $w = 1.0$. These deviations become more noticeable in testing with average prescribed strain levels closer to zero, as will be seen shortly.

4.4.1.2 Varying Prescribed Strain Amplitude

To assess the effects of varying strain amplitude the initial conditions will remain the same as the varying average strain test with the exception being the prescribed strain rate, $\bar{D}_{ii}$. The average strain level investigated is 0.0812 with the amplitudes being 0.015, 0.01 and 0.005. The three prescribed strain rates for these cases and the associated accumulated strains can be seen in Figures 4.19 and 4.20 respectively.

In light of the results of the previous section only the spheroidal void case is presented here and the results can be seen in Figure 4.21. As expected the void fractions are seen to increase with increased number of cycles, with the stronger rate of increase being seen for larger amplitudes. It should be noted that void coalescence will occur at void fractions much smaller than those observed here. The fact that the PCZ model, in its present form, doesn't account for void coalescence results in these elevated values of void volume fraction. Examining the distribution of voids assumed by the PCZ model a critical value of void fraction at coalescence of $\approx 52.36\%$ can be calculated, Appendix A. However, it should be noted that accounting for void

coalescence is much more detailed than simply applying this condition. The onset of coalescence will effect the overall behaviour of the material thus requiring the constitutive relations to be reevaluated at this condition. Regardless, since the major concern of these tests was to examine the overall behaviour produced by the PCZ model, no attempt was made to introduce this limitation on void fraction in the model. In addition to the void fraction results, it can be seen that the PCZ model predicts decreasing aspect ratio as cyclic loading progresses. The hardening rate predicts the initial hardening zone followed by an increasing softening zone, as can be seen more clearly in Figures 4.22 and 4.23. It can be concluded that the strain amplitude has a more dramatic influence on the results of the PCZ model under cyclic loading than does the average strain level. This is by no means a revelation seeing as the values of the strain rate, $\bar{D}_{n,i}$, are different throughout each cycle, which is not seen in the average strain level tests.

4.4.1.3 Varying Prescribed Strain Amplitude with No Preloading Applied and Minimum Strain Level of Zero

For these tests the same initial conditions as those applied in the previous two subsection are used. The prescribed strain rate, $\bar{D}_{n,i}$, Figure 4.24, does not include an initial preloading section and produces accumulated strains which are totally in the tensile zone and can be seen in Figure 4.25. As with the previous section the prescribed amplitudes are 0.015, 0.01 and 0.005.

The results of these tests, Figure 4.26, are comparable to those obtained in the previous section without the minor influences of the preloading zone. However, a major exception is with regards to the smallest of the amplitudes under investigation, 0.005. These differences, in the results obtained for this amplitude for f , w , $\frac{|\bar{\sigma}_{11}|}{\sigma_y}$ and $\frac{H}{\sigma_y}$, can be seen in Figures 4.27, 4.28, 4.29, 4.30 and 4.31. These plots indicated an opposite trend over the loading history than that produced for the higher amplitudes. In Figure 4.26 it is apparent that for higher amplitudes the progression away from the case $w = 1.0$ is quite smooth. This is not the case for 0.005, which is supported by Figure 4.28, where it is seen that the aspect ratio fails to escape the buffer zone around $w = 1.0$, discussed in the previous chapter. This causes the other terms to be adversely effected. To asses whether this problem is limited to this value for strain amplitude additional tests were conducted at amplitudes of 0.004, 0.0055 and 0.006. The results of these tests, Figure 4.32, show that this problem indeed does effect smaller values and to a lesser extent larger values than the 0.005 amplitude, see Figure 4.32(d) for initial deviation in hardening rate for amplitudes of 0.0055 and 0.006. In order to be sure that these transitions in predicted behaviour are in fact not a characteristic of the PCZ model additional tests were conducted where a preloading section moved through the case were $w = 1.0$. Specifically, an average strain level of 0.0812 was used with very small amplitudes, 0.0001 and 0.00001. These tests produced no transition in predicted behaviour and hence it can confidently be concluded

that the erroneous results are due to the $w = 1.0$ condition. To alleviate this problem, as well as those observed for the loadings of the earlier section, a better estimation, such as a linear approximation, is needed in the future for calculations around $w = 1.0$.

4.4.2 Compressive Zone

A similar procedure as that outlined for the tests in the tensile zone was used for the compressive zone tests by assigning a compressive initial stress and modifying the prescribed strain rates, Figures 4.15 and 4.19, so as to produce negative average strain values.

The results for the varying average strain tests, for the spheroidal void case, can be seen in Figure 4.33, which predict similar trends to the tensile case. The major difference being, the magnitude of the values predicted, which are influenced by the preloading prescribed, and the hardening rates which are seen to be opposite due to the negative value of stress in this case. The results observed make the predictions for the spherical void case more appealing since there exists a decreasing void fraction. For the spheroidal void case there is an increase in void fraction observed under overall compressive loading. While this may seem improbable, it is difficult to say if this observed behaviour is acceptable or not since experimental void evolution results under such loading conditions are not readily available. The tests involving

varying strain amplitude produce results, Figure 4.34, 4.35 and 4.36, which are also similar to the tensile results, with the same noted exceptions as above.

The above observations show that the PCZ model predicts results, under cyclic loading, which for the most part, conform to expected trends. One notable exceptions can be made for cyclic loading in the tensile zone with spherical voids where a decrease in void fraction is observed.

4.5 PseudoInverse Tests

Due to time limitations, full testing of the PCZ model with the simulation code developed by the MRCO, was not undertaken. As a result the behaviour of the model, and the PseudoInverse procedure, could not be assessed in a practical application. As a substitute, it was decided that a strain rate vector, which would be maintained throughout the loading history, would be prescribed. The resulting tests, would be similar to the uniaxial tests presented earlier except for the use of the PseudoInverse procedure of PorousMaterial.cc. For both tensile and compressive loading the initial conditions were assumed to be: $\frac{|\bar{\sigma}_{11}|}{\sigma_y} = 0.8$, $w_{start} = 1.0$, $f_{start} = 0.15$ and $\nu = 0.5$.

The prescribed strain rates were assumed: (i) $\bar{D}_{11} = \bar{D}_{22} = -0.3\bar{D}_{33}$ and (ii) $\bar{D}_{11} = \bar{D}_{22} = -0.5\bar{D}_{33}$. The results of the tests were seen to follow similar trends to those of the direct implementation i.e. using $\dot{K}$. As a result only the tensile

tests will be presented here and can be seen in Figures 4.37 and 4.38 for spherical and spheroidal void cases respectively. It can be seen that these results do indeed look similar to those produced by the direct solution, recall Figures 4.2 and 4.4. There are some obvious differences in magnitude since the prescribed values are not entirely the same i.e. $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ in the pseudo inverse case. As a result it can be concluded, based on these rather limited observations, that the PseudoInverse procedure seems to produce acceptable results. It should be noted that a more in-depth analysis is required on this function, using the simulation code, before definite acceptance of the results are taken. This suggestion can be extended to the entire PCZ model since only limited loading conditions were examined in this thesis work.

Chapter 5

The objective of the current work was to (1) implement the PCZ model as a constitutive relation in an object oriented code which simulates various manufacturing processes and (2) analyze the behaviour of the model under different loading conditions, assessing its validity as a tool for predicting the behaviour of porous material. To fulfill this goal, the function `PorousMaterial.cc` was created to apply the PCZ constitutive model for two simplified void shapes: spherical and spheroidal. This function was then used to conduct tests to examine the effects of: Poisson's Ratio, initial stress, initial prescribed void type and cyclic loading, on the results predicted by the PCZ model. This chapter summarizes the major trends revealed during these tests and outlines areas requiring further work.

Conclusions

- The spheroidal void case predicts an increase and decrease in void fraction, under tensile and compressive loading respectively. This translates into softening behaviour in tension and hardening behaviour in compression.

- The introduction of the aspect ratio, the spheroidal void case, results in a secondary hardening rate component which competes with the void fraction component. With aspect ratios greater than unity both tensile and compressive loading result in hardening and softening behaviour with increasing and decreasing aspect ratios respectively. The same behaviour is predicted but with larger magnitudes for aspect ratios less than unity.
- Poisson's ratio does not effect the results predicted under the spherical void case. However, since it directly influences the aspect ratio evolution the results of the spheroidal void case are effected as the loading increases.
- Initial stress level does not effect the evolution of void fraction or aspect ratio. The result is similar competition between the two hardening rate components regardless of stress level. The stress levels do, however, effect the magnitude of the hardening rates.
- Due to the competitive nature of the hardening rate components the initial aspect ratio greatly influences the results obtained.

- The PCZ model fails to predict acceptable results under cyclic loading in the spherical void case with tensile average strain. This is primarily due to the observed decrease in void fraction.
- Cyclic loading, of spheroidal voids with tensile and compressive average strain level, predicts an increase in void fraction with a decrease in aspect ratio. This could correspond to an evolution of the spheroidal void into a flat "crack" with eventual void coalescence.
- Cyclic loading, of spherical voids with compressive average strain level, predicts a decrease in void fraction with a decrease in aspect ratio, corresponding to the onset of void collapse.
- During cyclic loading the strain amplitude has a greater influence on the results than the average strain. This corresponds to the greater variation of loading on each cycle.
- During cyclic loading the average strain does not influence the evolution of aspect ratio and void fraction, except for the initial loading to get to the desired level.

- The PseudoInverse procedure was introduced because the predicted mapping between stress rate and strain rate could not be inverted. Preliminary testing reveals that this procedure produces qualitatively similar results to those given by the direct solution. In the future a more detailed analysis should be conducted on this procedure with PorousMaterial.cc used in conjunction with the simulation code for manufacturing processes.

Future Work

- PorousMaterial.cc now conducts calculations for the simplified spherical and spheroidal void situations. To obtain a more realistic situation the procedure should be extended to take into account the case of general ellipsoidal voids. This would require a numerical integration procedure to calculate the Eshelby tensor for each time step. In addition a third hardening rate component would be introduced, further complicating the interaction observed.

- PorousMaterial.cc should be linked with a secondary constitutive relation which will predict the hardening in the matrix phase. The combination would lead to more realistic predictions of the overall observed behaviour of porous materials.
- The PCZ model is formulated by assuming a composite with two distinct phases; the matrix and the inclusions. In the case investigated in this work the latter phase is assumed to correspond to a void. However, the model could also be reevaluated with the inclusion phase corresponding to hard secondary particles. The resulting constitutive model would produce results for a material with uniform distribution of particles of a different material.

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Tables

Table 1.1: Stress field ahead of a crack tip for Mode I and Mode II in a linear elastic, isotropic material. [15]

	Mode I	Mode II
σ_x	$\frac{K_I}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \left[1 - \sin\left(\frac{\theta}{2}\right) \sin\left(\frac{3\theta}{2}\right)\right]$	$-\frac{K_{II}}{\sqrt{2\pi r}} \sin\left(\frac{\theta}{2}\right) \left[2 + \cos\left(\frac{\theta}{2}\right) \cos\left(\frac{3\theta}{2}\right)\right]$
σ_y	$\frac{K_I}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \left[1 + \sin\left(\frac{\theta}{2}\right) \sin\left(\frac{3\theta}{2}\right)\right]$	$\frac{K_{II}}{\sqrt{2\pi r}} \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \cos\left(\frac{3\theta}{2}\right)$
τ_{xy}	$\frac{K_I}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{3\theta}{2}\right)$	$\frac{K_{II}}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \left[1 - \sin\left(\frac{\theta}{2}\right) \sin\left(\frac{3\theta}{2}\right)\right]$
σ_z	0 (Plane Stress) $\nu(\sigma_x + \sigma_y)$ (Plane Strain)	0 (Plane Stress) $\nu(\sigma_x + \sigma_y)$ (Plane Strain)
τ_{xz}, τ_{yz}	0	0

ν is Poisson's ratio.

Table 1.2: Crack tip displacement fields for Mode I and Mode II in linear elastic material. [15]

	Mode I	Mode II
u_x	$\frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} \cos\left(\frac{\theta}{2}\right) \left[\kappa - 1 + 2 \sin^2\left(\frac{\theta}{2}\right) \right]$	$\frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} \sin\left(\frac{\theta}{2}\right) \left[\kappa + 1 + 2 \cos^2\left(\frac{\theta}{2}\right) \right]$
u_y	$\frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} \sin\left(\frac{\theta}{2}\right) \left[\kappa + 1 - 2 \cos^2\left(\frac{\theta}{2}\right) \right]$	$-\frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} \cos\left(\frac{\theta}{2}\right) \left[\kappa - 1 - 2 \sin^2\left(\frac{\theta}{2}\right) \right]$

μ is the shear modulus

$\kappa = 3 - 4\nu$ (plane strain)

$\kappa = (3 - \nu)/(1 + \nu)$ (plane stress)

Table 1.3: Non-zero stress and displacement components in Mode III for linear elastic, isotropic material.[15]

$\tau_{xz} = -\frac{K_{III}}{\sqrt{2\pi r}} \sin\left(\frac{\theta}{2}\right)$
$\tau_{yz} = \frac{K_{III}}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right)$
$u_z = \frac{K_{III}}{\mu} \sqrt{\frac{r}{2\pi}} \sin\left(\frac{\theta}{2}\right)$

Figures

Figure 1.1: Potential Energy and Force as a function of atomic separation (after [10]).

Figure 1.2: Elliptical hole in a flat plate (after [10]).

Figure 1.3: Definition of the coordinate axis ahead of crack tip (after [10]).

Figure 1.4: The three modes of loading that can be applied to a crack.

Figure 1.5: Stress normal to the crack plane in Mode I (after [10]).

Figure 1.6: Through-thickness crack in an infinite plate subjected to remote tensile stress (after [10]).

Figure 1.7: First-order and second-order estimates of the plastic zone size, r_y and r_p respectively (after [10]).

(a)

(b)

Figure 1.8: The Strip Yield Model (after [10]).

Figure 1.9: Dimple formation owing to: uniaxial tensile loading shear and tensile tearing. (after [11]).

Figure 1.10: Schematic of crack extension by transgranular microvoid coalescence (after [11]).

Figure 1.11: Cylindrical void considered by McClintock [12].

a

b

Figure 1.12: Doubly periodic array of voids, (a), and an isolated cell, (b), considered by Needleman [23] to analyze numerically the effects of voids on material behaviour.

Figure 1.13: Results obtained by Needleman [23] for (a) Load versus strain for pure material and material with different sizes of initial voids and (b) The growth of the plastic zone (shaded area) and void under increasing overall strain. Note: the length L_0 becomes $U + L_0$ in the deformed body, thus $\frac{U}{L_0}$ is a measure of strain.

a

b

c

Figure 1.14: Representation proposed by Abeyaratne and Triantafyllidis [24] for (a) The cross section of the material, (b) the cross section of the unit cell and (c) the finite element grid of the unit cell.

Figure 2.1: Void geometry and distribution. (after [35]).

Figure 3.1: Plot of h as a function of aspect ratio, w , in close proximity and including the case where $w=1$.

Figure 3.2: Plot of h as a function of aspect ratio, w , excluding the case where $w=1$.

Figure 3.3: Flow chart showing interaction between PorousMaterial.cc and the upper level simulation code.

Figure 3.4: Flow chart showing major calculation steps involved in application of the PCZ model.

Figure 4.1: Results, presented by Ponte Castaneda and Zaidman [35], for uniaxial tension and compression of porous materials with initially isotropic distribution of spherical voids in 15% volume fraction. (a) Evolution of the void volume fraction; (b) evolution of the aspect ratio; (c) uniaxial stress-strain relation; (d) evolution of the effective hardening rate. The PCZ model is labeled, in the figure, as HS for spheroidal voids and HS $w = 1.0$ for spherical voids. Results obtained, for the same loading conditions, by the Gurson model [14], GS, were also included by Ponte Castaneda and Zaidman [35].

Figure 4.2: Results obtained from PorousMaterial.cc to compare with those of Ponte Castaneda and Zaidman [35], for the evolution of: f , $|\bar{\sigma}_N|/\sigma_y$, and H/σ_y under initial uniaxial tensile loading, $|\bar{\sigma}_N|/\sigma_y = 0.8$. The material had an initial isotropic distribution of spherical voids in 15% volume fraction and the voids were constrained to remain spherical.

Figure 4.3: Results obtained from PorousMaterial.cc to compare with those of Ponte Castaneda and Zaidman [35], for the evolution of: f , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under initial uniaxial compressive loading, $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. The material had an initial isotropic distribution of spherical voids in 15% volume fraction and the voids were constrained to remain spherical.

Figure 4.4: Results obtained from PorousMaterial.cc to compare with those of Ponte Castaneda and Zaidman [35], for the evolution of: f , w , $\bar{\sigma}_{33}/\sigma_y$, and H/σ_y under initial uniaxial tensile loading, $\bar{\sigma}_{33}/\sigma_y = 0.8$. The material had an initial isotropic distribution of spherical voids in 15% volume fraction.

Figure 4.5: Results obtained from PorousMaterial.cc to compare with those of Ponte Castaneda and Zaidman [35], for the evolution of: f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under initial uniaxial compressive loading, $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. The material had an initial isotropic distribution of spherical voids in 15% volume fraction.

Figure 4.6: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under uniaxial tension with $\nu = 0.3, 0.35, 0.4, 0.45, 0.5$. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = 0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.7: Variation of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , with Poisson's Ratio under uniaxial tension at a strain of 50%. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = 0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.8: Variation of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , with Poisson's Ratio under uniaxial tension at a strain of 100%. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = 0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.9: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under uniaxial compression with $\nu = 0.3, 0.35, 0.4, 0.45, 0.5$. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = -0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.10: Variation of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , with Poisson's Ratio under uniaxial compression at a strain of -30%. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = -0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.11: Variation of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , with Poisson's Ratio under uniaxial compression at a strain of -70%. Initially, 15% fraction of spherical voids and a stress level $|\bar{\sigma}_{33}|/\sigma_y = 0.8$. $D_{33} = -0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.12: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under uniaxial compression with varying initial stress values. Initially, 15% fraction of spherical voids. $\nu = 0.5$ $D_{33} = -0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.13: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y under uniaxial tension with varying initial aspect ratio. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ $D_{33} = 0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.14: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , under uniaxial compression with varying initial aspect ratio. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, -0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ $D_{33} = -0.01$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.15: Prescribed strain rate, D_{A} , for the case of cyclic loading in the tensile zone with average strain levels of: 0.1597, 0.0812 and 0.0340.

Figure 4.16: Accumulated strain during cyclic loading in the tensile zone with average strain levels of: 0.1597, 0.0812 and 0.0340.

Figure 4.17: Change observed in f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the tensile zone, with average strain levels of: 0.1597, 0.0812 and 0.0340. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. Spherical voids are maintained, $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.18: Change observed in f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the tensile zone, with average strain levels of: 0.1597, 0.0812 and 0.0340. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.19: Prescribed strain rate, D_{30} , for the case of cyclic loading in the tensile zone with strain amplitudes of: 0.015, 0.01 and 0.005.

Figure 4.20: Accumulated strain during cyclic loading in the tensile zone with strain amplitudes of: 0.015, 0.01 and 0.005

Figure 4.21: Changes observed in f , w , $|\bar{\sigma}_M|/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the tensile zone, with strain amplitudes of: 0.015, 0.01 and 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.22: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the tensile zone, with strain amplitudes of: 0.01 and 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0, 0, 0.8\sigma_y, 0, 0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.23: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the tensile zone, with a strain amplitude of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.24: Prescribed strain rate, D_{AV} , for the case of cyclic loading in the tensile zone with no prescribed preloading and an average strain rate level of zero. With strain amplitudes of: 0.015, 0.01 and 0.005.

Figure 4.25: Accumulated strain during cyclic loading in the tensile zone with no prescribed preloading and an average strain rate level of zero. With strain amplitudes of: 0.015, 0.01 and 0.005.

Figure 4.26: Changes observed in f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the tensile zone, with no prescribed preloading and minimum strain level zero and strain amplitudes of: 0.015, 0.01 and 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.27: Changes observed in void fraction, f , through 10,000 loading cycles, in the tensile zone, with with no prescribed preloading and minimum strain level of zero and a strain amplitude of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$, $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.28: Changes observed in aspect ratio, w , through 10,000 loading cycles, in the tensile zone no prescribed preloading and minimum strain level of zero and a strain amplitude of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.29: Changes observed in stress, $|\bar{\sigma}_{33}|/\sigma_y$, through 10,000 loading cycles, in the tensile zone, with no prescribed preloading and minimum strain level of zero and a strain amplitude of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$, $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.30: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the tensile zone, no prescribed preloading and minimum strain level of zero and strain amplitudes of: 0.01 and 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0.0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.31: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the tensile zone, with no prescribed preloading and minimum strain level of zero and a strain amplitudes of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0, 0, 0.8\sigma_y, 0, 0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.32: Changes observed in f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the tensile zone, with no prescribed preloading and minimum strain level of zero and strain amplitudes of: 0.004, 0.005, 0.0055 and 0.006. Initially, 15% fraction of spherical voids and stress vector, $\{0, 0, 0.8\sigma_y, 0, 0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.33: Change observed in f , w , $\bar{\sigma}_{33}/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the compressive zone, with average strain levels of: -0.1597, -0.0812 and -0.0340. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, -0.8\sigma_y, 0, 0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.34: Changes observed in f , w , $\bar{\sigma}_{x1}/\sigma_y$, and H/σ_y , through 10,000 loading cycles, in the compressive zone, with strain amplitudes of: 0.015, 0.01 and 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, -0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.35: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the compressive zone, with a strain amplitude of: 0.01. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, -0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.36: Changes observed in hardening rate, H/σ_y , through 10,000 loading cycles, in the compressive zone, with a strain amplitude of 0.005. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, -0.8\sigma_y, 0.0, 0\}$. $\nu = 0.5$ and $\bar{\sigma}_{11} = \bar{\sigma}_{22} = 0$ throughout.

Figure 4.37: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , as predicted using the PseudoInverse function of PorousMaterial.cc, under uniaxial tension. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. Two different sets of prescribed strain rates: (i) $D_{11} = D_{22} = -0.3D_{33}$ and (ii) $D_{11} = D_{22} = -0.5D_{33}$ are assumed throughout, along with $\nu = 0.5$. Spherical voids are maintained.

Figure 4.38: Evolution of f , w , $|\bar{\sigma}_{33}|/\sigma_y$, and H/σ_y , as predicted using the PseudoInverse function of PorousMaterial.cc, under uniaxial tension. Initially, 15% fraction of spherical voids and stress vector, $\{0.0, 0.8\sigma_y, 0.0, 0\}$. Two different sets of prescribed strain rates: (i) $D_{11} = D_{22} = -0.3D_{33}$ and (ii) $D_{11} = D_{22} = -0.5D_{33}$ are assumed throughout, along with $\nu = 0.5$. Spheroidal voids are maintained.

Appendices

Appendix A: Additional Information

(1) Definition of The Eshelby Tensor [36].

The Eshelby Tensor, S_{ijkl} , was developed to map the strain, which an elliptical inclusion would undergo in the absence of the matrix, to the actual strain observed when the void is constrained by the matrix. The tensor will have the same properties as the elastic coefficients of an orthorhombic crystal, with its axis parallel to the axis of the ellipsoid, though relations of the form $S_{1122} = S_{2211}$ are not valid. Coefficients coupling an extension and a shear ($S_{1112}, S_{1123}, S_{2311}, \dots$) or one shear to another ($S_{1223}, S_{2123}, \dots$) are zero. This corresponds to 15 independent components of the Eshelby Tensor:

$$\begin{array}{ccc} S_{1111} & S_{2222} & S_{3333} \\ S_{1122} & S_{2211} & S_{3311} \\ S_{1133} & S_{2233} & S_{3322} \\ S_{1212} & S_{2121} & S_{3131} \\ S_{1313} & S_{2323} & S_{3232} \end{array}$$

which are defined as follows:

$$\begin{aligned}
S_{1111} &= Qa^2 I_{aa} + RI_a \\
S_{1122} &= Qb^2 I_{bb} - RI_b \\
S_{1212} &= Q\frac{1}{2}(a^2 + b^2)I_{ab} + R\frac{1}{2}(I_a + I_b)
\end{aligned}$$

$$Q = \frac{3}{8\pi(1-\nu)}, \quad R = \frac{1-2\nu}{8\pi(1-\nu)}$$

$$I_a = 2\pi abc \int_0^\pi \frac{du}{(a^2 + u)\Delta}$$

$$I_{aa} = 2\pi abc \int_0^\pi \frac{du}{(a^2 + u)^2 \Delta}$$

where

$$I_{ab} = \frac{2}{3}\pi abc \int_0^\pi \frac{du}{(a^2 + u)(b^2 + u)\Delta}$$

$$\Delta = \sqrt{a^2 + u}\sqrt{b^2 + u}\sqrt{c^2 + u}$$

where a, b, c are the semi-axis lengths of the elliptical inclusion and ν is the matrix Poisson's ratio.

The remaining coefficients are found by simultaneous cyclic interchange of (1,2,3) and (a,b,c) in the above equations.

Since the Eshelby Tensor relates one strain tensor to another, $\varepsilon_{ij} = S_{ijkl}\varepsilon_{kl}$, some simplifications can be made:

$$(1) \quad S_{ijkl} = S_{jikl} \quad - \text{from the symmetry of the } \varepsilon_{kl} \text{ tensor.}$$

(2) $S_{\mu\lambda} = S_{\lambda\mu}$ - from the symmetry of the ε_y tensor.

This reduces $S_{\mu\lambda}$ to 36 independent components and to simplify calculations we will write $S_{\mu\lambda}$ as a 6x6 matrix (similar to that done with the elasticity tensor). Recalling the additional restrictions imposed by Eshelby, the 15 independent components take the form:

$$S_{\mu\lambda} = \begin{bmatrix} S_{1111} & S_{1122} & S_{1133} & 0 & 0 & 0 \\ S_{2211} & S_{2222} & S_{2233} & 0 & 0 & 0 \\ S_{3311} & S_{3322} & S_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2121} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{3131} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{3232} \end{bmatrix}$$

1.1 Spherical Voids

Since for spherical voids, $a = b = c = \text{radius}$, the independent components of $S_{\mu\lambda}$ are greatly reduced:

$$S_{\mu\lambda} = \begin{bmatrix} S_{1111} & S_{1122} & S_{1122} & 0 & 0 & 0 \\ S_{1122} & S_{1111} & S_{1122} & 0 & 0 & 0 \\ S_{1122} & S_{3322} & S_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2121} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{2121} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{2121} \end{bmatrix}$$

where

$$S_{1111} = \frac{7-5\nu}{15(1-\nu)}$$

$$S_{1122} = \frac{5\nu-1}{15(1-\nu)}$$

$$S_{1212} = \frac{4-5\nu}{15(1-\nu)}$$

1.2 Spheroidal Voids

In this case, we will assume that the major loading axis will correspond to the axis having the semi-axis length equal to a . The following will be developed for the major axis being the 33-direction in order to conform to the equations given by the PCZ model. However, in the PorousMaterial.cc function EshelbyTensor, modifications are made to account for other major axis directions. With these simplifications, the Eshelby Tensor is:

$$S_{ijkl} = \begin{bmatrix} S_{1111} & S_{1122} & S_{1133} & 0 & 0 & 0 \\ S_{1122} & S_{1111} & S_{1133} & 0 & 0 & 0 \\ S_{1133} & S_{1122} & S_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{2222} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{2121} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{2121} \end{bmatrix}$$

where

$$S_{1111} = \frac{3a^3b^2}{4(1-\nu)}(INT\#2) + \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#1)$$

$$S_{\Sigma\Sigma} = \frac{3ab^4}{4(1-\nu)}(INT\#5) + \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#4)$$

$$S_{\Sigma\Sigma\Sigma} = \frac{ab^4}{4(1-\nu)}(INT\#5) - \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#4)$$

$$S_{\Sigma\Sigma 11} = \frac{a^3b^2}{4(1-\nu)}(INT\#3) - \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#4)$$

$$S_{11\Sigma\Sigma} = \frac{ab^4}{4(1-\nu)}(INT\#3) - \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#1)$$

$$S_{\Sigma\Sigma\Sigma\Sigma} = \frac{ab^4}{4(1-\nu)}(INT\#5) + \frac{(1-2\nu)ab^2}{4(1-\nu)}(INT\#4)$$

$$S_{\Sigma\Sigma\Sigma\Sigma} = \frac{ab^2(b^2 + a^2)}{8(1-\nu)}(INT\#3) + \frac{(1-2\nu)ab^2}{8(1-\nu)}(INT\#4 + INT\#1)$$

and

$$INT\#1 = \frac{-2}{a(a^2 - b^2)} + \frac{\pi\sqrt{-1/(a^2 - b^2)}}{a^2 - b^2} + \frac{2\tanh^{-1}(a/\sqrt{a^2 - b^2})}{(a^2 - b^2)^{3/2}}$$

$$INT\#2 = \frac{-2(4a^2 - b^2)}{3a^3(a^2 - b^2)^2} + \frac{\pi\sqrt{-1/(a^2 - b^2)}}{(a^2 - b^2)^2} + \frac{2\tanh^{-1}(a/\sqrt{a^2 - b^2})}{(a^2 - b^2)^{3/2}}$$

$$INT\#3 = \frac{a^2 + 2b^2}{ab^2(a^2 - b^2)^2} - \frac{3\pi\sqrt{-1/(a^2 - b^2)}}{2(a^2 - b^2)^2} - \frac{3\tanh^{-1}(a/\sqrt{a^2 - b^2})}{(a^2 - b^2)^{3/2}}$$

$$INT\#4 = \frac{a}{a^2b^2 - b^4} - \frac{\pi\sqrt{-1/(a^2 - b^2)}}{2(a^2 - b^2)} - \frac{\tanh^{-1}(a/\sqrt{a^2 - b^2})}{(a^2 - b^2)^{3/2}}$$

$$INT\#5 = \frac{-(a(-2a^2 + 5b^2))}{4b^4(a^2 - b^2)^2} + \frac{3\pi\sqrt{-1/(a^2 - b^2)}}{8(a^2 - b^2)^2} + \frac{3\tanh^{-1}(a/\sqrt{a^2 - b^2})}{4(a^2 - b^2)^{3/2}}$$

In order to accommodate the situations when negative values occur under a square root and the results obtained from $\tanh^{-1}(x)$, the function EshelbyTensor performs calculations using complex variables for spheroidal voids. However, complex.h does not support a function for $\tanh^{-1}(x)$. To remedy this problem the following representation was used:

$$\tanh^{-1}(x) = \frac{1}{2} \ln \left(\frac{1+x}{1-x} \right); \quad |x| < 1.0$$

The condition $|x| < 1.0$ limits the use of this representation to cases where $b > a$ since in our case $x = \frac{a}{\sqrt{a^2 - b^2}}$. However, examining the results of $\tanh^{-1}(x)$ and the above representation with a graphing program revealed that when $|x| > 1.0$ i.e. $a > b$ the results have the same real part but the imaginary components are of opposite sign. As a result, this correction was hard coded directly into PorousMaterial.cc in the function ATANH which implements the above representation for $\tanh^{-1}(x)$.

2) Values of the Variables q_i ($i = 1..5$), from Ponte Castaneda & Zaidman[35]

The variables q_i ($i = 1..5$) appearing in Equation (2.18) for Q^2 , for the case of spheroidal inclusions, i.e. aspect ratio $= w = w_1 = w_2$, and porosity f are given by:

$$q_1 = 1 + \frac{2f(h + 2w^2 - 4hw^2)}{\Delta}$$

$$q_2 = 2 + \frac{f(6 - 5h - 4w^2 + 2hw^2)}{\Delta}$$

$$q_3 = 3 + \frac{12f(1 - w^2)(h + 2w^2 - 4hw^2)}{(1 - f)(4 - 3h - 2w^2)}$$

$$q_4 = 3 + \frac{6f(1 - w^2)}{(1 - f)(3h - 4w^2 + 3hw^2)}$$

$$q_5 = -1 - \frac{f(2h - 2w^2 + hw^2)}{\Delta}$$

$$\Delta = (1 - f)(2 - 3h)(h + 2w^2 - hw^2)$$

$$h = \frac{w \left[\cos^{-1}(w) - w\sqrt{1 - w^2} \right]}{(1 - w^2)^{3/2}}, \quad \text{if } w < 1$$

$$= \frac{w \left[-\cosh^{-1}(w) + w\sqrt{w^2 - 1} \right]}{(w^2 - 1)^{3/2}}, \quad \text{if } w > 1$$

(3) The Hardening Rate Function for Spheroidal Voids

The assumed hardening rate, for spheroidal voids, was expected to be:

$$H = - \left[(1-f) \frac{\delta \tilde{\Phi}}{\delta f} \frac{\delta \tilde{\Phi}}{\delta \bar{\sigma}_{kk}} + \left(w \frac{\delta \tilde{\Phi}}{\delta w} \right) \left(2A_{33ij}^{(2)} - A_{11ij}^{(2)} - A_{22ij}^{(2)} \right) \frac{\delta \tilde{\Phi}}{\delta \bar{\sigma}_{ij}} \right] \quad (A)$$

However, after initial testing and comparison of the obtained results to that of Ponte Castaneda and Zaidman [35] it was concluded that the actual form is:

$$H = - \left[(1-f) \frac{\delta \tilde{\Phi}}{\delta f} \frac{\delta \tilde{\Phi}}{\delta \bar{\sigma}_{kk}} + \left[\left(w \frac{\delta \tilde{\Phi}}{\delta w} \right) \left(2A_{33ij}^{(2)} - A_{11ij}^{(2)} - A_{22ij}^{(2)} \right) \frac{\delta \tilde{\Phi}}{\delta \bar{\sigma}_{ij}} \right] / 2 \right] \quad (B)$$

Which can possibly be explained if one takes into account the symmetry of the strain intensity tensor, $A_{ijkl}^{(2)}$. The inverse of the strain intensity tensor is calculated in terms of the Eshelby tensor (see Equation 2.22 and `InvStrIntensityTensor` in `PorousMaterial.cc`) and when inverted (`FormInverseMatrix` in `PorousMaterial.cc`) exhibits symmetry which produces:

$$A_{33ij}^{(2)} - A_{11ij}^{(2)} = A_{33ij}^{(2)} - A_{22ij}^{(2)} \quad (C)$$

Examining Equations B and C together, the result is that only one term associated with the aspect ratio contributes to the hardening rate. Thus it can be concluded that since the aspect ratios are the same, for spheroidal voids, the hardening rate need only take into account the aspect ratio contribution once hence the 1/2 factor in Equation B.

(4) Function: TimeIntegration

This function is required by all constitutive relations to be used in the casting simulation code. The simulation code has defined an enum constant type `StressType` which is assigned a value of either `ELASTIC`, `PLASTIC` or `INVALID`, depending on what deformation conditions are prevalent during the time step under consideration. During application of the PCZ model the variable will always contain the value `PLASTIC` except when the initial stress vector is the zero vector. In which case the calculations in the PCZ model cannot be conducted and the loading condition will be `ELASTIC` and an elastic constitutive relation using the isotropic elasticity tensor will be implemented.

(5) Possible Method To Account for Void Coalescence in the PCZ Model

As was presented in Figure 2.1 the PCZ model was developed such that the distribution of the voids in the porous material follow the same distribution as the void shape itself, i.e. $w_1 = \frac{l_1}{L_1} = \frac{L_1}{L_1}$ and $w_2 = \frac{l_2}{L_2} = \frac{L_2}{L_2}$. Where l_i $i = 1..3$ correspond to the void semi-axis lengths, a, b, c in PorousMaterial.cc, and L_i $i = 1..3$ are the spacings between the void centres. The following will examine one "cell" L_1 by L_2 by L_3 , consisting of an individual void and its surrounding matrix. From this representation a condition for void coalescence will be found for spherical and spheroidal voids.

5.1 Spherical Voids

In the spherical void case the cell will have the proportions $L_1 = L_2 = L_3$. The volume of the cell is given by:

$$V_{cell} = V_{matrix} + V_{void} = L_1^3 \quad (A)$$

The volume of the void is:

$$V_{void} = \frac{4}{3}\pi r^3 \quad (B)$$

The void volume fraction is given by:

$$f = \frac{V_{void}}{V_{cell}} \quad (C)$$

We can assume that void coalescence will occur when the following condition is met:

$$\frac{L_1}{2} = a \quad (D)$$

Substituting Equations (A) and (B) into (D) produces:

$$\frac{V_{cell}}{8} = \frac{3}{4\pi} V_{void} \quad (E)$$

Using Equation C the void volume fraction at coalescence is given by:

$$f_{coalescence} = \frac{\pi}{6} = 0.5236 \quad (F)$$

Therefore void coalescence will occur at $\approx 52.36\%$ void volume fraction.

5.2 Spheroidal Voids

In the spheroidal case the cell will have the properties $L_1 = L_2 = L_3$ and the void is seen to have $b = c = a$. The volume of the cell will be given by:

$$V_{cell} = V_{matrix} + V_{void} = L_3 L_1^2 \quad (G)$$

The volume of the void will be:

$$V_{void} = \frac{4}{3} \pi a b^2 \quad (H)$$

and the void volume fraction is again given by Equation C. For this void type two cases were investigated for void coalescence (i) for $w > 1.0$ and (ii) for $w < 1.0$. However, both cases produced the same critical value for the void volume fraction at coalescence. For this reason only the $w > 1.0$ case is presented here.

The condition for void coalescence is:

$$\frac{L_1}{2} = a \quad (I)$$

Substituting Equations (G) and (H) into (I) produces:

$$\frac{V_{cell}}{2L_2^2} = \frac{3}{4\pi h^2} V_{void} \quad (J)$$

Using Equation C the void volume fraction at coalescence is given by:

$$f_{coalescence} = \frac{2\pi h^2}{3L_2^2} \quad (K)$$

Using the definition of the aspect ratios, which have the same magnitude for the void and void distribution, produces:

$$f_{coalescence} = \frac{2\pi a^2}{3L_3^2} \quad (L)$$

Using the condition for coalescence, Equation (I):

$$f_{coalescence} = \frac{2\pi}{3} (0.25) = 0.5236 \quad (M)$$

This is the same critical value of void volume fraction at coalescence as that seen for the spherical void case. To implement this check for coalescence, the material's void volume fraction should be compared to this critical value at the end of each time step. If the observed void fraction is equal to or in excess of this critical value the material can be considered to have failed. It should be noted that void coalescence will greatly affect the constitutive behaviour

observed. For this reason this check should only be used as a limiting value on void fraction to eliminate unrealistic values of void fraction. If it is to be used as a true extension of the PCZ model then the constitutive relations should be reevaluated to capture the effects of coalescence.

Appendix B: PorousMaterial.cc

```
#include <math.h>
#include <complex.h>
#include <stdio.h>
#include "meschach.h"
#include "constitutive_model.h"

/***** POROUS MATERIAL MODEL (PCZ Model) *****/
/***** SIMPLIFIED FOR *****/
/***** SPHERICAL AND SPHEROIDAL VOIDS *****/
/***** BASED ON THE MODEL DEVELOPED BY *****/
/***** P. PONTE CASTANEDA AND M. ZAIDMAIN [1994]*****/

//constructor
/* The upper level code will pass PorousMaterial.cc the relevant
   information needed to conduct its calculations.

       props ->    vector of properties associated with the
                   material being considered

       iv ->      vector of internal variables required by the
                   constitutive model to conduct calculations

       sstart ->   principal stress vector at time of the call to the
                   constitutive model

       defGrad ->  deformation gradient, associated with the principal
                   directions, at the time of the call to the constitutive
                   model

       dt ->       time step under considerations */

PorousMaterial::PorousMaterial(VEC *props,double *iv,VEC *sstart,
                                MAT *defGrad, double dt):CauchyStress(props,iv,sstart,defGrad,dt)
{
    /***** PROPERTIES *****/
    youngsModulus = v_entry(props,0);
    poissonRatio  = v_entry(props,1);
    yieldStress   = v_entry(props,3);
}
```



```

/***** INTERNAL VARIABLES *****/

f_start      =   iv[23];      /* The void volume fraction at
*/              the beginning of the time step

VoidType     =   iv[24];      /* The void type to be
                              maintained: 1-spherical
                              2-spheroidal */

if (VoidType!=1 && VoidType!=2) { /* ERROR in value of
                              VoidType */

    printf ("\nThe constitutive model PorousMaterial\n");
    printf ("cannot produce valid results for the\n");
    printf ("void specification given. InternalVariable[24]\n");
    printf ("can only have the values 1 or 2 corresponding\n");
    printf ("to spherical and spheroidal voids respectively\n");
}

AxisLengtha_start =   iv[25];      /* Semi-axis length in the
                                  largest principal direction */
AxisLengthb_start =   iv[26];
AxisLengthc_start =   iv[27];      /* Semi-axis length in the other
                                  two principal directions */

LoadingFlag    =   iv[28];      /* Flag which defines the
                                  loading condition prescribed.
                                  Basically, this feature was added
                                  to control testing and may or
                                  may not be included if this
                                  model is used in practice.
                                  Values include:

                                  1: loading with principal strain
                                  rate in the 11 direction
                                  prescribed in addition to the
                                  principal stress rates in the 22 &
                                  33 directions

                                  2: loading with principal strain
                                  rate in the 22 direction
                                  prescribed in addition to the
                                  principal stress rates in the 11 &
                                  33 directions

```

3: loading with principal strain rate in the 33 direction prescribed in addition to the principal stress rates in the 11 & 22 directions

4: loading with principal stress rates in all three directions prescribed

5: loading condition where all three principal strain rate values are prescribed and calculations involve the pseudo-inverse. When implemented in practice this condition will use the deformation gradient to calculate the strain rates to be used with the pseudo-inverse */

```
if (LoadingFlag!=1 && LoadingFlag!=2 && LoadingFlag!=3 &&
    LoadingFlag!=4 && LoadingFlag!=5) { /* ERROR in value
                                         of LoadingFlag */
```

```
    printf ("\nThe constitutive model PorousMaterial\n");
    printf ("cannot produce valid results for the\n");
    printf ("loading condition specified.\n");
    printf ("InternalVariables[28] can only have the/nvalues:\n");
    printf ("\t1:\tuniaxial loading D11, dsig22dt, dsig33dt given\n");
    printf ("\t2:\tuniaxial loading D22, dsig11dt, dsig33dt given\n");
    printf ("\t3:\tuniaxial loading D33, dsig22dt, dsig11dt given\n");
    printf ("\t4:\tdsig11dt, dsig22dt, dsig33dt given\n");
    printf ("\t5:\tApproximation using pseudo-inverse\n");
```

```
}
```

```
PrescribedValue1 = iv[29];
PrescribedValue2 = iv[30];
PrescribedValue3 = iv[31]; /* The prescribed principal
                             stress or strain rates as defined
                             for various loadings by
                             LoadingFlag */
```

```
CumStrain = iv[32]; /* Accumulated strain, used for
                     testing purposes only */
```

```

f_end      = f_start;    /* Void volume fraction at the
                           end of the time step */

w_start    = AxisLengtha_start/AxisLengthb_start;
                           /* Aspect ratio of
                           the voids
                           calculated from the
                           semi-axis lengths */
}
/*****/

//destructor

PorousMaterial::~PorousMaterial()
{
}

/*****/
/* Function: TimeIntegration

This function is required by all constitutive relations by the file,
constitutive_model.h . It will assign a value of either ELASTIC or PLASTIC
depending on the value of the variable, regime, which reflects the
deformation type. If the value of regime is not as expected then a value of
INVALID is returned*/

TStressType PorousMaterial::TimeIntegration(int regime)
{
    if (regime == 0) {
        return ELASTIC;
    }

    else if (regime == 1) {
        return PLASTIC;
    }

    else {

```

```

        return INVALID;
    }
}

/*****
/* Function: FormDynStiff

    This function receives the values of:

        stress ->    principal stress vector at the beginning of the
                     time step

        B ->        matrix which maps principal stress vector
                     onto the vector representing the rate of
                     change of the yield function, phi, with
                     change in principal stress

        H ->        hardening rate for time step

```

and uses these values to produce Kdot, the mapping of principal stress rate vector onto principal strain rate vector. */

```

MAT *PorousMaterial::FormDynStiff(VEC *stress,MAT *B,double H)
{

```

```

    MAT *StressSquared,*Intermediate1,*Intermediate2,*Kdot;

```

```

    StressSquared = m_get(6,6);

```

```

    StressSquared->me[0][0] = pow(stress->ve[0],2.);

```

```

    StressSquared->me[1][1] = pow(stress->ve[1],2.);

```

```

    StressSquared->me[2][2] = pow(stress->ve[2],2.);

```

```

    StressSquared->me[0][1] = stress->ve[0]*stress->ve[1];

```

```

    StressSquared->me[0][2] = stress->ve[0]*stress->ve[2];

```

```

    StressSquared->me[1][0] = StressSquared->me[0][1];

```

```

    StressSquared->me[1][2] = stress->ve[1]*stress->ve[2];

```

```

    StressSquared->me[2][0] = StressSquared->me[0][2];

```

```

    StressSquared->me[2][1] = StressSquared->me[1][2];

```

```

    Intermediate1 = m_get(6,6);

```

```

    sm_mlt((1./H),B,Intermediate1);

```

```

    Intermediate2 = m_get(6,6);

```

```

    m_mlt(Intermediate1,StressSquared,Intermediate2);

```

```

Kdot = m_get(6,6);
mmtr_mlt(Intermediate2,B,Kdot);

m_free(StressSquared);
m_free(Intermediate1);
m_free(Intermediate2);

return Kdot;
}

```

```

/*****
/* Function: B_Matrix

```

This function receives the values of:

w ->	void aspect ratio
f ->	void volume fraction
ystress ->	yield stress of the matrix material
majoraxis ->	flag defining which of the three principal directions is the primary loading axis
voidtype ->	flag defining which void type (spherical or spheroidal) is to be maintained, the value of which dictates which calculations are performed

and uses them to produce the matrix, B, which maps principal stress vector onto the vector representing the rate of change of the yield function, phi, with change in principal stress */

```

MAT *PorousMaterial::B_Matrix(double w,double f,double yStress,
                             double majoraxis,double voidtype)
{
    MAT *B;
    double a,b,c,q1,q2,q3,q5,delt,h,k1;

    double epsilon= 1.0e-4;    /* Used as a tolerance around on the
                                value of aspect ratio, w=1.0, to avoid
                                the discontinuities observed in the
                                function, h, defined in P. PONTE

```

CASTANEDA AND M. ZAIDMAIN
[1994] for the spheroidal void case */

```

B = m_get(6,6);

if (voidtype==1.) { // Spherical Voids
    a = 1./6./pow((-1.+f),2.)/yStress;
    b = 12.-f;
    c = -6.+5.*f;

    // compose the matrix B
    B->me[0][0] = b*a;
    B->me[1][1] = b*a;
    B->me[2][2] = b*a;
    B->me[3][3] = 1.;
    B->me[4][4] = 1.;
    B->me[5][5] = 1.;

    B->me[0][1] = c*a;
    B->me[0][2] = c*a;
    B->me[1][0] = c*a;
    B->me[1][2] = c*a;
    B->me[2][0] = c*a;
    B->me[2][1] = c*a;

    return B;
}

else if ((voidtype==2) || (w!=1.)) { //Spheroidal Voids
    if ((w<=1.0) && (w>(1.0-epsilon))) { /* Aspect ratio within
        tolerance but <=1.0 */
        w = w - epsilon;
    }

    else if ((w<(1.0+epsilon)) && (w>1.0)) { /* Aspect ratio within
        tolerance but >1.0 */
        w = w + epsilon;
    }
}

```

```

/* Variables h, delt, q1->q5 all defined in P. PONTE CASTANEDA
AND M. ZAIDMAIN [1994] */

if (w < 1.) {

    h = w*(acos(w) - w*pow((1. - pow(w,2)),1./2.))
        /pow((1. - pow(w,2)),3./2.);

}

else { // w>1

    h = w*(-acosh(w) + w*pow((pow(w,2) - 1.),1./2.))
        /pow((pow(w,2) - 1),3./2.);

}

k1 = 1./(1. - f)/yStress;

delt = (1. - f)*(2. - 3.*h)*(h + 2.*pow(w,2) - h*pow(w,2));

q1 = 1. + 2.*f*(h + 2.*pow(w,2) - 4.*h*pow(w,2))/delt;

q2 = 2. + f*(6. - 5.*h - 4.*pow(w,2) + 2.*h*pow(w,2))/delt;

q3 = 3. + 12.*f*(1. - pow(w,2)) * (h + 2.*pow(w,2) - 4.*h*pow(w,2))
    /(1. - f)/(4. - 3.*h - 2.*pow(w,2));

q5 = -1. - f*(2.*h - 2.*pow(w,2) + h*pow(w,2))/delt;

}

// compose the matrix B using the value of majoraxis to determine the
form

if (majoraxis==1.) {

    B->me[0][0] = k1*q2;
    B->me[1][1] = k1*(q1/2. + q3);
    B->me[2][2] = k1*(q1/2. + q3);
    B->me[3][3] = 1.;
    B->me[4][4] = 1.;
    B->me[5][5] = 1.;

    B->me[0][1] = k1*q5;
    B->me[0][2] = k1*q5;

```

```

        B->me[1][0] = k1*q5;
        B->me[1][2] = k1*(q1/2. - q3);
        B->me[2][0] = k1*q5;
        B->me[2][1] = k1*(q1/2. - q3);
    }

    else if (majoraxis==2)    {

        B->me[0][0] = k1*(q1/2. + q3);
        B->me[1][1] = k1*q2;
        B->me[2][2] = k1*(q1/2. + q3);
        B->me[3][3] = 1.;
        B->me[4][4] = 1.;
        B->me[5][5] = 1.;
        B->me[0][1] = k1*q5;
        B->me[0][2] = k1*(q1/2. - q3);
        B->me[1][0] = k1*q5;
        B->me[1][2] = k1*q5;
        B->me[2][0] = k1*(q1/2. - q3);
        B->me[2][1] = k1*q5;
    }

    else if (majoraxis==3)    {

        B->me[0][0] = k1*(q1/2. + q3);
        B->me[1][1] = k1*(q1/2. + q3);
        B->me[2][2] = k1*q2;
        B->me[3][3] = 1.;
        B->me[4][4] = 1.;
        B->me[5][5] = 1.;

        B->me[0][1] = k1*(q1/2. - q3);
        B->me[0][2] = k1*q5;
        B->me[1][0] = k1*(q1/2. - q3);
        B->me[1][2] = k1*q5;
        B->me[2][0] = k1*q5;
        B->me[2][1] = k1*q5;
    }

    return B;
}

/*****/

```


/* Function: HardeningRate

This function receives values for:

stress ->	principal stress vector at the beginning of the time step
f ->	void volume fraction
w ->	void aspect ratio
majoraxis ->	flag defining which of the three principal directions is the primary loading axis
ystress ->	yield stress of the matrix material
A ->	Strain intensity tensor
B ->	matrix which maps principal stress vector onto the vector representing the rate of change of the yield function, phi, with change in principal stress
voidtype ->	flag defining which void type (spherical or spheroidal) is to be maintained, the value of which dictates which calculations are performed

and calculates the value of the hardening rate during the time step. */

```
double PorousMaterial::HardeningRate(VEC *stress,double f,double w,
double majoraxis,double yStress,
MAT *A, MAT *B,double voidtype)
```

```
{
```

```
double epsilon= 1.0e-4; /* Used as a tolerance around on the value of
aspect ratio, w=1.0, to avoid the
discontinuities observed in the function, h,
defined in P. PONTE CASTANEDA AND M.
ZAIDMAIN [1994] for the spheroidal void
case */
```

```
double MajorStress,MinorStress1,MinorStress2,
```

```

k1,k2,q1,q2,q3,q5,dq1df,dq2df,dq3df,dq5df,
dq1dw,dq2dw,dq3dw,dq5dw,delt,ddeltdf,ddeltdw,
h,dhdw,dphidf,dphidw,H;

```

```

VEC  *dphidsig,*Rowa,*Rowb,*Rowc,*Rowa_b,*Rowa_c;

```

```

dphidsig = v_get(6);
mv_mlt(B,stress,dphidsig);

```

```

Rowa = v_get(6);
Rowb = v_get(6);
Rowc = v_get(6);
Rowa_b = v_get(6);
Rowa_c = v_get(6);          /* Rows and combinations of rows of A,
                             which are used in the spheroidal calculations
                             of hardening rate, H */

```

```

if (voidtype==1.) {        //Spherical Void

```

```

    dphidf = (1./12.)*(-23.*pow(stress->ve[0],2.)
        +14.*stress->ve[0]*stress->ve[1]
        -23.*pow(stress->ve[1],2.)+14.*stress->ve[1]*stress->ve[2]
        -23.*pow(stress->ve[2],2.)+14.*stress->ve[2]*stress->ve[0]
        -10.*stress->ve[0]*stress->ve[1]*f
        -10.*stress->ve[1]*stress->ve[2]*f
        -10.*stress->ve[2]*stress->ve[0]*f
        +pow(stress->ve[0],2.)*f
        +pow(stress->ve[1],2.)*f
        +pow(stress->ve[2],2.)*f)/(pow((-1.+f),3.)*yStress);

```

```

    H = -((1.-f)*dphidf*(dphidsig->ve[0]+dphidsig->ve[1]
        +dphidsig->ve[2]));

```

```

}

```

```

else if ((voidtype==2) || (w!=1.)) {        //Spheroidal Void

```

```

    /* Assigning values to variables which depend on the primary
    loading axis */

```

```

    if (majoraxis==1.) {

```

```

        get_row(A,0,Rowa);
        get_row(A,1,Rowb);
        get_row(A,2,Rowc);
    }

```

```

MajorStress = stress->ve[0];
MinorStress1 = stress->ve[1];
MinorStress2 = stress->ve[2];
}

else if (majoraxis==2.) {

    get_row(A,1,Rowa);
    get_row(A,2,Rowb);
    get_row(A,0,Rowc);

    MajorStress = stress->ve[1];
    MinorStress1 = stress->ve[2];
    MinorStress2 = stress->ve[0];

}

else if (majoraxis==3.) {

    get_row(A,2,Rowa);
    get_row(A,0,Rowb);
    get_row(A,1,Rowc);

    MajorStress = stress->ve[2];
    MinorStress1 = stress->ve[0];
    MinorStress2 = stress->ve[1];

}

v_sub(Rowa,Rowb,Rowa_b);
v_sub(Rowa,Rowc,Rowa_c);

if ((w<=1.0) && (w>(1.0-epsilon))) { /* Aspect ratio
                                      within tolerance
                                      but <=1.0 */

    w = w - epsilon;

}

else if ((w<(1.0+epsilon)) && (w>1.0)) { /* Aspect ratio
                                           within tolerance
                                           but >1.0 */

    w = w + epsilon;

```

```

}

/* Variables h, delt, q1->q5 all defined in P. PONTE
CASTANEDA AND M. ZAIDMAIN [1994] */

if (w < 1.) {

    h = w*(acos(w) - w*pow((1. - pow(w,2)),1./2.))
        / pow((1. - pow(w,2)),3./2.);

    /* Derivative of h wrt aspect ratio, w */

    dhdw = (acos(w) - w*pow((1. - pow(w,2)),1./2.))
        / pow((1. - pow(w,2)),3./2.)
        + w*(-1./pow((1. - pow(w,2)),1./2.)
        - pow((1. - pow(w,2)),1./2.) + pow(w,2)
        / pow((1. - pow(w,2)),1./2.))
        / pow((1. - pow(w,2)),3./2.)
        + 3.*pow(w,2)*acos(w)
        - w*pow((1. - pow(w,2)),1./2.))
        / pow((1. - pow(w,2)),5./2.);

}

else { // w > 1

    h = w*(-acosh(w) + w*pow((pow(w,2) - 1.),1./2.))
        / pow((pow(w,2) - 1.),3./2.);

    dhdw = (-acosh(w) + w*pow((pow(w,2) - 1.),1./2.))
        / pow((pow(w,2) - 1.),3./2.)
        + w*(-1./pow((pow(w,2) - 1.),1./2.)
        + pow((pow(w,2) - 1.),1./2.) + pow(w,2)
        / pow((pow(w,2) - 1.),1./2.))
        / pow((pow(w,2) - 1.),3./2.)
        - 3.*pow(w,2)
        * (-acosh(w) + w*pow((pow(w,2) - 1.),1./2.))
        / pow((pow(w,2) - 1.),5./2.);

}

k1 = 1./(1. - f)/yStress;
k2 = 1./pow((1. - f),2)/yStress;

```

```

delt = (1. - f)*(2. - 3.*h)*(h + 2.*pow(w,2) - h*pow(w,2));
/* Derivative of delt wrt void volume fraction, f */
ddeltdf = -(2. - 3.*h)*(h + 2.*pow(w,2) - h*pow(w,2));
/* Derivative of delt wrt aspect ratio, w */
ddeltdw = -3.*(1. - f)*dhdw*(h + 2.*pow(w,2) - h*pow(w,2))
          + (1. - f)*(2. - 3.*h)*(dhdw + 4.*w - dhdw*pow(w,2)
          - 2.*h*w);
q1 = 1. + 2.*f*(h + 2.*pow(w,2) - 4.*h*pow(w,2))/delt;
q2 = 2. + f*(6. - 5.*h - 4.*pow(w,2) + 2.*h*pow(w,2))/delt;
q3 = 3. + 12.*f*(1. - pow(w,2)) * (h + 2.*pow(w,2) - 4.*h*pow(w,2))
      / (1. - f)/(4. - 3.*h - 2.*pow(w,2));
q5 = -1. - f*(2.*h - 2.*pow(w,2) + h*pow(w,2))/delt;
/* Derivative of q1->q5 wrt void volume fraction, f */
dq1df = 2.*(h + 2.*pow(w,2) - 4.*h*pow(w,2))/delt
        - 2.*f*(h + 2.*pow(w,2) -
        4.*h*pow(w,2))*ddeltdf/pow(delt,2);
dq2df = (6. - 5.*h - 4.*pow(w,2) + 2.*h*pow(w,2))/delt
        - f*(6. - 5.*h - 4.*pow(w,2)
        + 2.*h*pow(w,2))*ddeltdf/pow(delt,2);
dq3df = 12.*(1. - pow(w,2)) * (h + 2.*pow(w,2) - 4.*h*pow(w,2))
        / (1. - f)/(4. - 3.*h - 2.*pow(w,2))
        + 12.*f*(1. - pow(w,2)) * (h + 2.*pow(w,2)
        - 4.*h*pow(w,2))
        / pow((1. - f),2)/(4. - 3.*h - 2.*pow(w,2));
dq5df = -(2.*h - 2.*pow(w,2) + h*pow(w,2))/delt
        + f*(2.*h - 2.*pow(w,2) + h*pow(w,2))*ddeltdf/pow(delt,2);
/* Derivative of q1->q5 wrt aspect ratio, w */
dq1dw = 2.*f*(dhdw + 4.*w - 4.*dhdw*pow(w,2) - 8.*h*w)/delt
        - 2.*f*(h + 2.*pow(w,2)
        - 4.*h*pow(w,2))*ddeltdw/pow(delt,2);

```

```

dq2dw = f*(-5.*dhdw - 8.*w + 2*dhdw*pow(w,2) + 4.*h*w)/delt
        - f*(6. - 5.*h - 4.*pow(w,2)
        + 2.*h*pow(w,2))*ddeltdw/pow(delt,2);
dq3dw = -24.*f*w*(h + 2.*pow(w,2) - 4.*h*pow(w,2))
        /(1. - f)/(4. - 3.*h - 2.*pow(w,2))
        + 12.*f*(1. - pow(w,2))*(dhdw + 4.*w
        - 4.*dhdw*pow(w,2)
        - 8.*h*w)/(1. - f)/(4. - 3.*h - 2.*pow(w,2))
        - 12.*f*(1. - pow(w,2))*(h + 2.*pow(w,2)
        - 4.*h*pow(w,2))
        * (-3.*dhdw - 4.*w)/(1. - f)/pow((4. - 3.*h
        - 2.*pow(w,2)),2);

dq5dw = -f*(2.*dhdw - 4.*w + dhdw*pow(w,2) + 2.*h*w)/delt
        + f*(2.*h - 2.*pow(w,2)
        + h*pow(w,2))*ddeltdw/pow(delt,2);

/* Derivative of the yield function, phi, wrt void volume
fraction, f */
dphidf = k1*(dq1df*1./4.*pow((MinorStress1 + MinorStress2),2)
        + 1./2.*dq2df*pow(MajorStress,2)
        + dq3df*1./2.*pow((MinorStress1 - MinorStress2),2)
        + 2.*dq5df*1./2.*(MinorStress1
        + MinorStress2)*MajorStress)
        + k2*(q1*1./4.*pow((MinorStress1
        + MinorStress2),2)
        + 1./2.*q2*pow(MajorStress,2)
        + q3*1./2.*pow((MinorStress1 - MinorStress2),2)
        + 2.*q5*1./2.*(MinorStress1
        + MinorStress2)*MajorStress);

/* Derivative of the yield function, phi, wrt aspect ratio, w */
dphidw = k1*(dq1dw*1./4.*pow((MinorStress1
        + MinorStress2),2)
        + 1./2.*dq2dw*pow(MajorStress,2)
        + dq3dw*1./2.*pow((MinorStress1 -
        MinorStress2),2)
        + 2.*dq5dw*1./2.*(MinorStress1
        + MinorStress2)*MajorStress);

H = -((1-f)*dphidf*(dphidsig->ve[0] + dphidsig->ve[1]
        + dphidsig->ve[2])
        + (w*dphidw*(dphidsig->ve[0]*Rowa_b->ve[0]
        + dphidsig->ve[1]*Rowa_b->ve[1]

```

```

+ dphidsig->ve[2]*Rowa_b->ve[2])
+ w*dphidw*(dphidsig->ve[0]*Rowa_c->ve[0]
+ dphidsig->ve[1]*Rowa_c->ve[1]
+ dphidsig->ve[2]*Rowa_c->ve[2]))/2.);
}

v_free(dphidsig);
v_free(Rowa);
v_free(Rowb);
v_free(Rowc);
v_free(Rowa_b);
v_free(Rowa_c);

return H;
}

/*****
/* Function: CalcPseudoInverse

This function takes the matrix, kdot, which is not invertable by
conventional means since det=0, and calculates its pseudo-inverse as outlined
in:
    Strang, G. "Linear Algebra and Its Applications",
    Academic Press, Inc. New York, New York, 1976.    */

MAT *PorousMaterial::CalcPseudoInverse(MAT *kdot)
{
    int i,j;
    double epsilon=MACHEPS;
    MAT *U,*V,*A,*APLUS,*SIGMAPLUS,*Intermediate,*PseudoInverse;
    VEC *svdvals;

    /* An (m x n) matrix A can undergo a singular value decomposition
    such that:


$$A = U^T \text{SIGMA } V$$


    where
    A:      an (m x n) matrix
    U:      an (m x m) orthogonal matrix
    V:      an (n x n) orthogonal matrix
    SIGMA:  diagonal matrix with positive
            numbers in the first r-entries and zero
            otherwise

```

The non-zero diagonal values of SIGMA correspond to the singular values, u_i . Subsequently, the pseudo-inverse, APLUS, can be defined as:

$$\text{APLUS} = V^T \text{SIGMAPLUS} U$$

where SIGMAPLUS is also a diagonal matrix with entries $1/u_i$. In practice it is essential to find very small values of u_i , which may arise due to round off errors etc. during the decomposition, and set them equal to zero. If this is not done these values will transform into unwanted large values in SIGMAPLUS. A good tolerance to check u_i is 100 times the machine epsilon (MACHEPS). */

```
A = m_get(3,3);
```

```
/* Since the only part of the (6 x 6) matrix kdot which is not invertable
is the fully populated upper-left (3 x 3) then only the pseudo-inverse of
this section will be taken. */
```

```
for(i = 0; i<3; i++) {
    for(j = 0; j<3; j++)
        A->me[i][j] = kdot->me[i][j];
}
```

```
U = m_get(3,3);
V = m_get(3,3);
svdvals = v_get(3);
svd(A,U,V,svdvals);
```

```
/* Since the function svd() puts the singular values in vector form we
must form SIGMAPLUS, first checking the size of the singular values
against the tolerance selected */
```

```
for(i = 0; i<3; i++) {
    if (svdvals->ve[i] < (100*epsilon)) {
        svdvals->ve[i]=0;
    }
}
```

```
SIGMAPLUS = m_get(3,3);
for(i = 0; i<3; i++) {
    for(j = 0; j<3; j++) {
        if ((i==j) && svdvals->ve[i]!=0) {
            SIGMAPLUS->me[i][j] = 1./svdvals->ve[i];
        }
    }
}
```



```

    }
}

Intermediate = m_get(3,3);
mtrm_mlt(V,SIGMAPLUS,Intermediate);

APLUS = m_get(3,3);
m_mlt(Intermediate,U,APLUS);

/* Composing the entire pseudo-inverse for the (6 x 6) matrix kdot */
PseudoInverse = m_get(6,6);

PseudoInverse->me[0][0] = APLUS->me[0][0];
PseudoInverse->me[1][1] = APLUS->me[1][1];
PseudoInverse->me[2][2] = APLUS->me[2][2];
PseudoInverse->me[3][3] = 1.;
PseudoInverse->me[4][4] = 1.;
PseudoInverse->me[5][5] = 1.;

PseudoInverse->me[0][1] = APLUS->me[0][1];
PseudoInverse->me[0][2] = APLUS->me[0][2];
PseudoInverse->me[1][0] = APLUS->me[1][0];
PseudoInverse->me[1][2] = APLUS->me[1][2];
PseudoInverse->me[2][0] = APLUS->me[2][0];
PseudoInverse->me[2][1] = APLUS->me[2][1];

v_free(svdvals);
m_free(U);
m_free(V);
m_free(A);
m_free(SIGMAPLUS);
m_free(Intermediate);
m_free(APLUS);

return PseudoInverse;
}

/*****
/* Function: FormInverseMatrix

This function calculates the inverse of a (6 x 6) matrix, initial */
MAT *PorousMaterial::FormInverseMatrix(MAT *initial)

```

```

{
    double det;
    MAT *inverse;
    int i,j;

    inverse = m_get(6,6);

    det = (initial->me[0][0]*(initial->me[1][1]*initial->me[2][2]
        -initial->me[2][1]*initial->me[1][2])
        -initial->me[1][0]*(initial->me[0][1]*initial->me[2][2]
        -initial->me[2][1]*initial->me[0][2])
        +initial->me[2][0]*(initial->me[0][1]*initial->me[1][2]
        -initial->me[1][1]*initial->me[0][2]));

    for(i = 0; i<6; i++)
        for(j = 0; j<6; j++) {
            if(i==0 && j==0)
                inverse->me[i][j] += ((initial->me[1][1]
                    *initial->me[2][2]
                    -initial->me[2][1]
                    *initial->me[1][2])/det);

            if(i==0 && j==1)
                inverse->me[i][j] += ((initial->me[0][2]
                    *initial->me[2][1]
                    -initial->me[0][1]
                    *initial->me[2][2])/det);

            if(i==0 && j==2)
                inverse->me[i][j] += ((initial->me[0][1]
                    *initial->me[1][2]
                    -initial->me[1][1]
                    *initial->me[0][2])/det);

            if(i==1 && j==0)
                inverse->me[i][j] += ((initial->me[1][2]
                    *initial->me[2][0]
                    -initial->me[1][0]
                    *initial->me[2][2])/det);

            if(i==1 && j==1)
                inverse->me[i][j] += ((initial->me[0][0]
                    *initial->me[2][2]
                    -initial->me[2][0]
                    *initial->me[0][2])/det);

            if(i==1 && j==2)
                inverse->me[i][j] += ((initial->me[0][2]
                    *initial->me[1][0]
                    -initial->me[0][0]
                    *initial->me[1][2])/det);
        }
}

```

```

        if(i==2 && j==0)
            inverse->me[i][j] += ((initial->me[1][0]
                                   *initial->me[2][1]
                                   -initial->me[2][0]
                                   *initial->me[1][1])/det);
        if(i==2 && j==1)
            inverse->me[i][j] += ((initial->me[0][1]
                                   *initial->me[2][0]
                                   -initial->me[0][0]
                                   *initial->me[2][1])/det);
        if(i==2 && j==2)
            inverse->me[i][j] += ((initial->me[0][0]
                                   *initial->me[1][1]
                                   -initial->me[1][0]
                                   *initial->me[0][1])/det);
        if((i==3 && j==3) || (i==4 && j==4) || (i==5 && j==5))
            inverse->me[i][j] += 1./initial->me[i][j];
    }

    return inverse;
}

/*****
/* Function: ElasticityTensor

    This function uses Youngs Modulus (yModulus) and Poisson's
    Ratio (poissonR) to form the isotropic elasticity tensor (elasticity) */

MAT *PorousMaterial::ElasticityTensor(double yModulus,double poissonR )
{
    double a,b,c;
    MAT *elasticity;

    a = yModulus* (1. - poissonR)/(1. + poissonR)/(1. - 2.* poissonR);
    b = yModulus* poissonR/(1. + poissonR)/(1. - 2.* poissonR);
    c = yModulus/2./(1. + poissonR);

    //now compose elasticity_matrix

    elasticity = m_get(6,6);

    elasticity->me[0][0]=a;
    elasticity->me[1][1]=a;
    elasticity->me[2][2]=a;

```

```

elasticity->me[3][3]=c;
elasticity->me[4][4]=c;
elasticity->me[5][5]=c;

elasticity->me[0][1]=b;
elasticity->me[0][2]=b;
elasticity->me[1][0]=b;
elasticity->me[1][2]=b;
elasticity->me[2][0]=b;
elasticity->me[2][1]=b;

return elasticity;
}

/*****
/* Function: Linearization

This function receives:

    INCstress ->    the total stress increment predicted by
                    the constitutive relation during the
                    time step

    Strain ->      strain increment during time step

    yModulus ->    Young's Modulus

    poissonR ->    Poisson's Ratio

    elasticity ->  isotropic elasticity tensor

    stresstype ->  flag either ELASTIC or PLASTIC

and uses these values to calculate a linear approximation, D, to the stress-
strain behaviour predicted by the model */

MAT *PorousMaterial::Linearization(VEC *INCstress, VEC *Strain,
                                   double yModulus, double poissonR,
                                   MAT *elasticity, TStressType stresstype)
{
    double E12,E13,E23,Eavg,PRavg,a,b,c;
    double Etotal=0;
    double PRtotal=0; double counter=0;
    MAT *D;

```

```

D = m_get(6,6);

if (stresstype==ELASTIC) /* If the deformation is elastic then the linear
                           approximation is simply the isotropic
                           elasticity tensor */

    return m_copy(elasticity,D);

if (stresstype==PLASTIC) {

    /* Both the stress vector and the strain vector are known,
    therefor it is considered that the approximated linear mapping
    between the two will have a similar form as the elastic matrix.
    However, the values Young's Modulus (E) and Poisson's Ratio
    (PR) will be different from those of the elastic case. The elastic
    form gives:

        strain1 = stress1/E - PR*stress2/E - PR*stress3/E    (1)

        strain2 = -PR*stress1/E + stress2/E - PR*stress3/E    (2)

        strain3 = -PR*stress1/E - PR*stress2/E + stress3/E    (3)

    Solving (1) & (2) or (1) & (3) or (2) & (3) will produce different
    values of E & PR in the PLASTIC case. It is then proposed that
    the averages of these values (if they can be calculated) will be
    used as the modified Young's Modulus and Poisson's Ratio.*/

    // Solving (1) & (2)

    /*Condition when E and PR can not be calculated */

    if((Strain->ve[1]/Strain->ve[0]) == ((INCstress->ve[0]
                                     +INCstress->ve[2])
                                     /(INCstress->ve[1]+INCstress->ve[2])))
    || (INCstress->ve[0]==INCstress->ve[1] &&
        INCstress->ve[0]==-INCstress->ve[2])
    || (Strain->ve[1]==Strain->ve[0] && Strain->ve[0]==0.)) {

    }

    else {
        counter += 1.;

        E12 = (INCstress->ve[1]*(INCstress->ve[1]
                                + INCstress->ve[2])

```

```

- INCstress->ve[0]*(INCstress->ve[0]
+ INCstress->ve[2]))
/(Strain->ve[1]*(INCstress->ve[1]
+ INCstress->ve[2]) - Strain->ve[0]*(INCstress->ve[0]
+ INCstress->ve[2]));

Etotal += E12;

PRtotal += (INCstress->ve[0] - E12*Strain->ve[0])/
(INCstress->ve[1] + INCstress->ve[2]);
}

// Solving (1) & (3)

/*Condition when E and PR can not be calculated */
if((Strain->ve[2]/Strain->ve[0]) == ((INCstress->ve[0]
+INCstress->ve[1])
/(INCstress->ve[1]+INCstress->ve[2]))
|| (INCstress->ve[0]==INCstress->ve[2] &&
INCstress->ve[0]==-INCstress->ve[1])
|| (Strain->ve[2]==Strain->ve[0] && Strain->ve[0]==0.)) {
}

else {
counter += 1.;

E13 = (INCstress->ve[2]*(INCstress->ve[1]
+ INCstress->ve[2])
- INCstress->ve[0]*(INCstress->ve[0]
+ INCstress->ve[1]))
/(Strain->ve[2]*(INCstress->ve[1]
+ INCstress->ve[2]) - Strain->ve[0]*(INCstress->ve[0]
+ INCstress->ve[1]));

Etotal += E13;

PRtotal += (INCstress->ve[0] - E13*Strain->ve[0])/
(INCstress->ve[1] + INCstress->ve[2]);
}

// Solving (2) & (3)

/*Condition when E and PR can not be calculated */

```

```

if((Strain->ve[2]/Strain->ve[1]) == ((INCstress->ve[1]
                                     +INCstress->ve[0])
                                     /(INCstress->ve[2]+INCstress->ve[0]))
|| (INCstress->ve[1]==INCstress->ve[2] &&
    INCstress->ve[1]==-INCstress->ve[0])
|| (Strain->ve[2]==Strain->ve[1] && Strain->ve[1]==0.)) {
}

else {
    counter += 1.;

    E23 = (INCstress->ve[2]*(INCstress->ve[0]
        + INCstress->ve[2])
        - INCstress->ve[1]*(INCstress->ve[1]
        + INCstress->ve[0]))/(Strain->ve[2]*(INCstress->ve[0]
        + INCstress->ve[2]) - Strain->ve[1]*(INCstress->ve[1]
        + INCstress->ve[0]));

    Etotal += E23;

    PRtotal += (INCstress->ve[1] - E23*Strain->ve[1])/
        (INCstress->ve[0] + INCstress->ve[2]);
}

if(counter==0.) { /* If none of the modified values for E
                  and PR could be calculated then the
                  best approximation will be the elastic
                  values */

    Eavg = yModulus;
    PRavg = poissonR;

}

else { /* Modified E and PR */

    Eavg = Etotal/counter;
    PRavg = PRtotal/counter;

}

/* Calculating the components of the linear approximation */
a = Eavg*(1. - PRavg)/(1. + PRavg)/(1. - 2.* PRavg);
b = Eavg* PRavg/(1. + PRavg)/(1. - 2.* PRavg);

```

```

        c = yModulus/2./(1. + poissonR);

        //now compose the matrix D

        D->me[0][0]=a;
        D->me[1][1]=a;
        D->me[2][2]=a;
        D->me[3][3]=c;
        D->me[4][4]=c;
        D->me[5][5]=c;

        D->me[0][1]=b;
        D->me[0][2]=b;
        D->me[1][0]=b;
        D->me[1][2]=b;
        D->me[2][0]=b;
        D->me[2][1]=b;

        return D;
    }

    return MNULL;
}

/*****
/* Function: InvStrIntensityTensor

    This function receives values for the Eshelby Tensor (eshelby)
    and void volume fraction (f) and calculates the inverse of the strain intensity
    tensor as defined by the PCZ model */

MAT *PorousMaterial::InvStrIntensityTensor(MAT *eshelby,double f)
{
    double a;
    MAT *Unity,*invA;
    int i,j;

    a = -(1-f);

    /* Get a (6 x 6) identity matrix */
    Unity = m_get(6,6);

```



```

m_ident(Unity);

invA = m_get(6,6);
ms_mltadd(Unity,eshelby,a,invA);

m_free(Unity);

return invA;
}

/*****
/* Function: EshelbyTensor

This function will take the Poisson's Ratio (poissonR) the semi-
axis lengths: a,b (only these two are needed since for spherical voids a=b=c and
for spheroidal voids b=c) and the flag majoraxis and subsequently forms the
Eshelby Tensor (Eshelby) as defined in:

Eshelby, J.D. (1957) "The Deformation of the Elastic Field
of an Ellipsoidal Inclusion, and Related Problems"
Proc. R. Soc. Lond. A 241, 376-396. */

MAT *PorousMaterial::EshelbyTensor(double poissonR,double a,double b,
double majoraxis)
{
double Pi = 3.141592654;
double w,S1111,S1122,S2211,S2222,S2233,S2121,S3232;

complex acomp(a),bcomp(b); /* Complex form used since
spheroidal calculations involve
hyperbolic tangent function */

complex INT1,INT2,INT3,INT4,INT5;
MAT *Eshelby;

w=a/b;

if (w==1.) { /*Spherical void

/* Calculation of the independent components of the Eshelby
Tensor */

S1111 = (7. - 5.*poissonR)/(15.*(1. - poissonR));
S3232 = (4. - 5.*poissonR)/(15.*(1. - poissonR));

```

```

S1122 = (5.*poissonR - 1.)/(15.*(1. - poissonR));

// now compose the Eshelby Tensor for spherical voids

Eshelby = m_get(6,6);

Eshelby->me[0][0] = S1111;
Eshelby->me[1][1] = S1111;
Eshelby->me[2][2] = S1111;
Eshelby->me[3][3] = S3232;
Eshelby->me[4][4] = S3232;
Eshelby->me[5][5] = S3232;

Eshelby->me[0][1] = S1122;
Eshelby->me[0][2] = S1122;
Eshelby->me[1][0] = S1122;
Eshelby->me[1][2] = S1122;
Eshelby->me[2][0] = S1122;
Eshelby->me[2][1] = S1122;

}

else if (w>1. || w<1.) { //Spheroidal void

/* Calculation of the integrals which are used in the
independent components of the Eshelby Tensor */

INT1 = -2./acompp/(pow(acompp,2)-pow(bcompp,2))
+ Pi*pow((-1./(pow(acompp,2)-pow(bcompp,2))),1./2.)
/(pow(acompp,2)-pow(bcompp,2))
+ 2.*ATANH(acompp,bcompp)
/pow((pow(acompp,2)-pow(bcompp,2)),3./2.);

INT2 = -2.*(4.*pow(acompp,2)-pow(bcompp,2))/3./pow(acompp,3)
/pow((pow(acompp,2)-pow(bcompp,2)),2)
+ Pi*pow((-1./(pow(acompp,2)-pow(bcompp,2))),1./2.)
/pow((pow(acompp,2)-pow(bcompp,2)),2)
+ 2.*ATANH(acompp,bcompp)
/pow((pow(acompp,2)-pow(bcompp,2)),5./2.);

INT3 = (pow(acompp,2)+2.*pow(bcompp,2))/acompp/pow(bcompp,2)
/pow((pow(acompp,2)-pow(bcompp,2)),2)
- 3.*Pi*pow((-1./(pow(acompp,2)-pow(bcompp,2))),1./2.)
/2./pow((pow(acompp,2)-pow(bcompp,2)),2)

```

```

- 3.*ATANH(acomp,bcomp)
/pow((pow(acomp,2)-pow(bcomp,2)),5./2.);

INT4 = acomp/(pow(acomp,2)*pow(bcomp,2)-pow(bcomp,4))
- Pi*pow((-1./ (pow(acomp,2)-pow(bcomp,2))),1./2.)
/2./ (pow(acomp,2)-pow(bcomp,2))
- ATANH(acomp,bcomp)
/pow((pow(acomp,2)-pow(bcomp,2)),3./2.);

INT5 = -acomp*(-2.*pow(acomp,2)+5.*pow(bcomp,2))
/4./pow(bcomp,4)
/pow((pow(acomp,2)-pow(bcomp,2)),2)
+ 3.*Pi*pow((-1./ (pow(acomp,2)-pow(bcomp,2))),1./2.)
/8./pow((pow(acomp,2)-pow(bcomp,2)),2)
+ 3.*ATANH(acomp,bcomp)
/4./pow((pow(acomp,2)-pow(bcomp,2)),5./2.);

// Constructing the independent components of the Eshelby
Tensor for Spheroidal voids

S1111 = 3.*pow(a,3)*pow(b,2)*real(INT2)/4./ (1.-poissonR)
+ (1.-2.*poissonR)*a*pow(b,2)*real(INT1)
/4./ (1.-poissonR);

S1122 = a*pow(b,4)*real(INT3)/4./ (1.-poissonR)
- (1.-2.*poissonR)*a*pow(b,2)*real(INT1)
/4./ (1.-poissonR);

S2211 = pow(a,3)*pow(b,2)*real(INT3)/4./ (1.-poissonR)
- (1.-2.*poissonR)*a*pow(b,2)*real(INT4)
/4./ (1.-poissonR);

S2222 = 3.*a*pow(b,4)*real(INT5)/4./ (1.-poissonR)
+ (1.-2.*poissonR)*a*pow(b,2)*real(INT4)
/4./ (1.-poissonR);

S2233 = a*pow(b,4)*real(INT5)/4./ (1.-poissonR)
- (1.-2.*poissonR)*a*pow(b,2)*real(INT4)
/4./ (1.-poissonR);

S2121 = a*pow(b,2)*(pow(a,2)+pow(b,2))*real(INT3)
/8./ (1.-poissonR)
+ (1.-2.*poissonR)*a*pow(b,2)
*(real(INT4)+real(INT1))
/8./ (1.-poissonR);

```

```

S3232 = a*pow(b,4)*real(INT5)/4./(1.-poissonR)
      + (1.-2.*poissonR)*a*pow(b,2)*real(INT4)
      /4./(1.-poissonR);

//now compose the Eshelby Tensor for spherical voids with
various major loading axis

Eshelby = m_get(6,6);

if (majoraxis==1.) {

    Eshelby->me[0][0] = S1111;
    Eshelby->me[1][1] = S2222;
    Eshelby->me[2][2] = S2222;
    Eshelby->me[3][3] = S2121;
    Eshelby->me[4][4] = S2121;
    Eshelby->me[5][5] = S3232;

    Eshelby->me[0][1] = S1122;
    Eshelby->me[0][2] = S1122;
    Eshelby->me[1][0] = S2211;
    Eshelby->me[1][2] = S2233;
    Eshelby->me[2][0] = S2211;
    Eshelby->me[2][1] = S2233;

}

else if (majoraxis==2.) {

    Eshelby->me[0][0] = S2222;
    Eshelby->me[1][1] = S1111;
    Eshelby->me[2][2] = S2222;
    Eshelby->me[3][3] = S2121;
    Eshelby->me[4][4] = S3232;
    Eshelby->me[5][5] = S2121;

    Eshelby->me[0][1] = S2211;
    Eshelby->me[0][2] = S2233;
    Eshelby->me[1][0] = S1122;
    Eshelby->me[1][2] = S1122;
    Eshelby->me[2][0] = S2233;
    Eshelby->me[2][1] = S2211;

}

else if (majoraxis==3.) {

```

```

Eshelby->me[0][0] = S2222;
Eshelby->me[1][1] = S2222;
Eshelby->me[2][2] = S1111;
Eshelby->me[3][3] = S3232;
Eshelby->me[4][4] = S2121;
Eshelby->me[5][5] = S2121;

```

```

Eshelby->me[0][1] = S2233;
Eshelby->me[0][2] = S2211;
Eshelby->me[1][0] = S2233;
Eshelby->me[1][2] = S2211;
Eshelby->me[2][0] = S1122;
Eshelby->me[2][1] = S1122;

```

```

}

```

```

}

```

```

return Eshelby;

```

```

}

```

```

/*****
/* Function: ATANH

```

This function was constructed in light of the fact that complex.h does not support a function for $\tanh^{-1}$. To remedy this problem the following representation was used:

$$\tanh^{-1} = (1/2) \ln((1+x)/(1-x)); \quad |x| < 1.0$$

The condition $|x| < 1.0$ limits the use of this equation to the case where $b > a$ since in our case $x = a / (((a^2) - (b^2))^{1/2})$. However, examining the results of $\arctanh(x)$ and the representation $(1/2) \ln((1+x)/(1-x))$ with a graphing program revealed that when $|x| > 1.0$ (ie) $a > b$ the results have the same real part but the imaginary components are of opposite sign. As a result this correction is hard coded into the function. */

```

complex PorousMaterial::ATANH(complex a,complex b)
{

```

```

    complex y,x,z;
    double v,w;

```

```

    x = a/pow((pow(a,2)-pow(b,2)),1./2.);

```

```

y = 1./2.*log((1.+x)/(1.-x));
v = real(y);
w = imag(y);
if (real(a) > real(b))    {
    complex i(v),j(0,-w);
    z = i + j;
}
else if (real(a) < real(b)) {
    z = y;
}
return z;
}

/*****
/* Function: VoidFractionUpdate

This function will use the strain rate vector (StrRt) and original
void volume fraction (f1) along with the time step (delt) to calculate the
updated void fraction (f2). */

double PorousMaterial::VoidFractionUpdate(VEC *StrRt,double f1,
double delt)
{
    double dfdt,temp,f2;

    /* Calculate the time derivative of void volume fraction */
    dfdt = (1. - f1)*(StrRt->ve[0] + StrRt->ve[1] + StrRt->ve[2]);
    temp = f1 + dfdt*delt;

    /* Condition to avoid negative void fractions */
    if(temp<=0)
        f2 = 0;
    else
        f2 = temp;
}

```

```

        return f2;
    }

    /*****
    /* Function: AxisUpdate

        This function uses the stress intensity tensor (A), strain rate
        vector (StrRt), time step (delt), original void semi-axis lengths (a1, b1, c1), the
        original and updated void volume fractions (f1 & f2), and the flags majoraxis
        and voidtype to conduct the calculations to update the void semi-axis lengths
        and enforce the void shape */

    VEC *PorousMaterial::AxisUpdate(MAT *A,VEC *StrRt,double delt,
                                   double a1,double b1,double c1,
                                   double f1,double f2,double majoraxis,
                                   double voidtype)
    {
        double w1=a1/b1;
        double w2=a1/c1;          /* Setting initial aspect ratios from initial
                                   semi-axis lengths */
        double dw1dt,dw2dt;
        double w1_new,w2_new,a2,b2,c2,NewAxisLength;
        VEC *Rowa,*Rowb,*Rowc,*Rowa_b,*Rowa_c,*AxisLengths_end;

        Rowa = v_get(6);
        Rowb = v_get(6);
        Rowc = v_get(6);
        Rowa_b = v_get(6);
        Rowa_c = v_get(6);        /* Rows and combinations of rows of A,
                                   which are used in the evolution calculations
                                   of hardening */

        /* Assigning values to rows as determined by the primary loading axis
    */

        if (majoraxis==1.) {
            get_row(A,0,Rowa);
            get_row(A,1,Rowb);
            get_row(A,2,Rowc);
        }
    }

```

```

else if (majoraxis==2.)    {

    get_row(A,1,Rowa);
    get_row(A,2,Rowb);
    get_row(A,0,Rowc);

}

else if (majoraxis==3.)    {

    get_row(A,2,Rowa);
    get_row(A,0,Rowb);
    get_row(A,1,Rowc);

}

v_sub(Rowa,Rowb,Rowa_b);
v_sub(Rowa,Rowc,Rowa_c);

/* Calculating the time rate of change of the aspect ratios */

dw1dt = w1*(Rowa_b->ve[0]*StrRt->ve[0]
    + Rowa_b->ve[1]*StrRt->ve[1]
    + Rowa_b->ve[2]*StrRt->ve[2]
    + Rowa_b->ve[3]*StrRt->ve[3]
    + Rowa_b->ve[4]*StrRt->ve[4] + Rowa_b->ve[5]*StrRt->ve[5]);

dw2dt = w2*(Rowa_c->ve[0]*StrRt->ve[0]
    + Rowa_c->ve[1]*StrRt->ve[1]
    + Rowa_c->ve[2]*StrRt->ve[2] + Rowa_c->ve[3]*StrRt->ve[3]
    + Rowa_c->ve[4]*StrRt->ve[4] + Rowa_c->ve[5]*StrRt->ve[5]);

/* Updating aspect ratios */

w1_new = w1 + dw1dt*delt;
w2_new = w2 + dw2dt*delt;

/* Updating the void semi-axis lengths */

if ((w1_new<=0) || (w2_new<=0) || (f2==0))    {    /* Condition
collapse                                     to signify
                                              void
                                              */

    a2 = 0;
    b2 = 0;

```



```

        c2 = 0;
    }

    else {

        a2 = pow((f2*w1_new*w2_new*a1*b1*c1/f1),(1./3.));
        b2 = a2/w1_new;
        c2 = a2/w2_new;
    }

    /* Since for the case of spheroidal voids the condition b=c must be
    maintained, we will let the new axis length "a" remain as calculated
    and use conservation of volume on the void to find a new length for
    the other two axis such that b=c. Similarly, for the spherical void case,
    a=b=c. */

    if (voidtype == 1.) { //Maintain spherical voids

        if (a2==0 || b2==0 || c2==0) { //Collapsed voids */
            NewAxisLength = 0;
        }

        else {
            NewAxisLength = pow((a2*b2*c2),(1./3.));
        }

        AxisLengths_end = v_get(3);
        AxisLengths_end->ve[0] = NewAxisLength;
        AxisLengths_end->ve[1] = NewAxisLength;
        AxisLengths_end->ve[2] = NewAxisLength;
    }

    else if (voidtype == 2.) { //Maintain spheroidal voids

        if (a2==0 || b2==0 || c2==0) { //Collapsed voids */
            NewAxisLength = 0;
        }

        else {
            NewAxisLength = sqrt(b2*c2);
        }

        AxisLengths_end = v_get(3);
        AxisLengths_end->ve[0] = a2;
        AxisLengths_end->ve[1] = NewAxisLength;

```

```

        AxisLengths_end->ve[2] = NewAxisLength;
    }

    v_free(Rowa_c);
    v_free(Rowa_b);
    v_free(Rowa);
    v_free(Rowb);
    v_free(Rowc);

    return AxisLengths_end;
}

```

```

/***** /
/* Function: ComputeStress

```

The upper level code will call this function to implement the porous material constitutive model and ComputeStress will subsequently control the calculations, calling functions internal to this constitutive model and returning the updated information to the calling program.

(i.e.) ResultStress -> will receive the updated principal stress vector at the end of the time step

ResultIntVariables -> will receive the updated internal variables such as: void volume fraction, void semi-axis lengths and hardening rate.

ResultD -> will receive a matrix which represents a linear approximation to the behaviour predicted by this constitutive model */

```

void PorousMaterial::ComputeStress(VEC **ResultStress,
                                   double **ResultIntVariables,
                                   MAT **ResultD)
{

```

```

    TStressType stressType; /* Variable required by
                             constitutive_model.h either ELASTIC
                             or PLASTIC */

```

```

int Regime;      /* Flag used to set stressType    0: ELASTIC
                                                         1: PLASTIC */

double H, MajorAxis, MAX, Det=1;

/*    H -> `hardening rate

    MajorAxis ->    variable used to
                    control calculations by
                    holding information on
                    which principal
                    direction is the major
                    loading direction

    MAX ->          variable used in
                    determining MajorAxis

    Det ->          required in call to the
                    function Strain() of
                    CauchyStress.cc which
                    calculates the strain
                    from the deformation
                    gradient. Not directly
                    used in this code. */

VEC  *strain, *StrainRate, *ElasticStress, *PorousStressRt, *PorousStress,
    *incStress, *finalStress, *new_axis_lengths, *PseudoStrRt;

/*    strain ->      principal strain vector
                    over time step

    StrainRate ->    principal strain rate
                    vector over time step

    ElasticStress -> elastic stress increment
                    vector over time step

    PorousStressRt -> porous stress rate vector
                    over time step

    PorousStress ->  porous stress increment
                    vector over time step

```

incStress ->	total (elastic + porous) stress increment vector over time step
finalStress ->	initial stress vector + total stress increment vector
new_axis_lengths ->	updated void semi-axis lengths
PseudoStrRt ->	strain rate used to calculate the updated void fraction and void semi-axis lengths when pseudo-inverse procedure is used */


```

MAT      *D,*Kdot,*elasticity,*Eshelby,*InvStrIntensity,*StrIntensity,*B,
      *Mapping,*PseudoInverse;
/*      D->          linear approximation to
                    the results predicted by t
                    he constitutive model

      Kdot->        matrix mapping
                    PorousStressRt onto
                    StrainRate

      elasticity->   isotropic elasticity tensor

      Eshelby->     Eshelby Tensor

      InvStrIntensity -> inverse of the strain
                        intensity tensor

      StrIntensity -> strain intensity tensor

      B->           matrix which maps
                    principal stress vector
                    onto the vector
                    representing the rate of
                    change of the yield
                    function, phi, with
                    change in principal stress

```

Mapping -> required in call to the function Strain() of CauchyStress.cc which calculates the strain from the deformation gradient. Not directly used in this code.

PseudoInverse-> pseudo-inverse of Kdot which is not invertable by conventional means i.e. its det=0 */

```
if ((VoidType==1 || VoidType==2) &&
    (LoadingFlag==1 || LoadingFlag==2 ||
    LoadingFlag==3 || LoadingFlag==4 ||
    LoadingFlag==5)) { /* Condition checking that all flages are valid
                        */
```

```
Mapping = m_get(3,3);
```

```
if ((pow(StressStart->ve[0],2) + pow(StressStart->ve[1],2)
+ pow(StressStart->ve[2],2))==0) { /* If initial stress values
are all zero the PCZ
model cannot be used
and hence for this time
step the elastic
constitutive relation will
be used */
```

```
Regime = 0; /* ELASTIC */
```

```
stressType = TimeIntegration(Regime);
```

```
/* Calculating strain from the deformation gradient */
strain = v_get(6);
Strain (Hencky,DeformationGradient,strain,Mapping,&Det);
```

```
elasticity = ElasticityTensor(youngsModulus,poissonRatio);
```

```
ElasticStress = v_get(6);
mv_mlt(elasticity,strain,ElasticStress);
```

```
finalStress = v_get(6);
v_add(StressStart,ElasticStress,finalStress);
```

```

D = Linearization(incStress,strain,youngsModulus,poissonRatio,
                  elasticity,stressType);

/* No changes in internal variables */

new_axis_lengths = v_get(3);
new_axis_lengths->ve[0] = AxisLengtha_start;
new_axis_lengths->ve[1] = AxisLengthb_start;
new_axis_lengths->ve[2] = AxisLengthc_start;

*ResultStress = v_copy(finalStress,VNULL);
*ResultD = m_copy(D,MNULL);

*ResultIntVariables = new double[4];
(*ResultIntVariables)[0] = f_end;
(*ResultIntVariables)[1] = new_axis_lengths->ve[0];
(*ResultIntVariables)[2] = new_axis_lengths->ve[1];
(*ResultIntVariables)[3] = new_axis_lengths->ve[2];

m_free(Mapping);
m_free(D);
m_free(elasticity);
v_free(finalStress);
v_free(ElasticStress);
v_free(strain);
v_free(new_axis_lengths);
}

else {

    Regime = 1;      /* PLASTIC */

    stressType = TimeIntegration(Regime);

    if (LoadingFlag != 5.) {      /* pseudo-inverse not used
                                (i.e.) direct solution using Kdot
                                */

        //Assign value to MajorAxis

        if (LoadingFlag==1. || LoadingFlag==2.
            || LoadingFlag==3.) {

            MajorAxis = LoadingFlag;

        }
    }
}

```

```

else if (LoadingFlag==4)    {
    MAX = fabs(PrescribedValue1);
    MajorAxis = 1.;

    if (MAX < fabs(PrescribedValue2))    {
        MAX = fabs(PrescribedValue2);
        MajorAxis = 2.;
    }

    if (MAX < fabs(PrescribedValue3));    {
        MAX = fabs(PrescribedValue3);
        MajorAxis = 3.;
    }
}

Eshelby = EshelbyTensor(poissonRatio,AxisLengtha_start,
                        AxisLengthb_start,MajorAxis);
InvStrIntensity = InvStrIntensityTensor(Eshelby,f_start);
StrIntensity = FormInverseMatrix(InvStrIntensity);

B = B_Matrix(w_start,f_start,yieldStress,
             MajorAxis,VoidType);
H = HardeningRate(StressStart,f_start,w_start,MajorAxis,
                  yieldStress,StrIntensity,B,VoidType);

Kdot = FormDynStiff(StressStart,B,H);

StrainRate = v_get(6);
PorousStressRt = v_get(6);

/* Direct calculations using
[StrainRate] = [Kdot] [PorousStressRt] */

if (LoadingFlag==1.)    {    // uniaxial loading:
                        // D11,dsig22dt,
                        // dsig33dt given

    StrainRate->ve[0] = PrescribedValue1;
    PorousStressRt->ve[1] = PrescribedValue2;

```

```

PorousStressRt->ve[2] = PrescribedValue3;

PorousStressRt->ve[0] = (StrainRate->ve[0]
    - Kdot->me[0][1]
    * PorousStressRt->ve[1]
    - Kdot->me[0][2]
    * PorousStressRt->ve[2])
    / Kdot->me[0][0];

StrainRate->ve[1] = Kdot->me[1][0]
    * PorousStressRt->ve[0]
    + Kdot->me[1][1]
    * PorousStressRt->ve[1]
    + Kdot->me[1][2]
    * PorousStressRt->ve[2];

StrainRate->ve[2] = Kdot->me[2][0]
    * PorousStressRt->ve[0]
    + Kdot->me[2][1]
    * PorousStressRt->ve[1]
    + Kdot->me[2][2]
    * PorousStressRt->ve[2];
}

else if (LoadingFlag==2.) { // uniaxial loading:
    // dsig11dt,D22,
    // dsig33dt given

PorousStressRt->ve[0] = PrescribedValue1;
StrainRate->ve[1] = PrescribedValue2;
PorousStressRt->ve[2] = PrescribedValue3;

PorousStressRt->ve[1] = (StrainRate->ve[1]
    - Kdot->me[1][0]
    * PorousStressRt->ve[0]
    - Kdot->me[1][2]
    * PorousStressRt->ve[2])
    / Kdot->me[1][1];

StrainRate->ve[0] = Kdot->me[0][0]
    * PorousStressRt->ve[0]
    + Kdot->me[0][1]
    * PorousStressRt->ve[1]
    + Kdot->me[0][2]
    * PorousStressRt->ve[2];

```



```

StrainRate->ve[2] = Kdot->me[2][0]
                    *PorousStressRt->ve[0]
                    + Kdot->me[2][1]
                    * PorousStressRt->ve[1]
                    + Kdot->me[2][2]
                    * PorousStressRt->ve[2];
}

else if (LoadingFlag==3.) { // uniaxial loading:
                          // dsig11dt,dsig22dt,
                          // D33 given

PorousStressRt->ve[0] = PrescribedValue1;
PorousStressRt->ve[1] = PrescribedValue2;
StrainRate->ve[2] = PrescribedValue3;

PorousStressRt->ve[2] = (StrainRate->ve[2]
                        - Kdot->me[2][0]
                        * PorousStressRt->ve[0]
                        - Kdot->me[2][1]
                        * PorousStressRt->ve[1])
                        /Kdot->me[2][2];

StrainRate->ve[0] = Kdot->me[0][0]
                    * PorousStressRt->ve[0]
                    + Kdot->me[0][1]
                    * PorousStressRt->ve[1]
                    + Kdot->me[0][2]
                    * PorousStressRt->ve[2];

StrainRate->ve[1] = Kdot->me[1][0]
                    * PorousStressRt->ve[0]
                    + Kdot->me[1][1]
                    * PorousStressRt->ve[1]
                    + Kdot->me[1][2]
                    * PorousStressRt->ve[2];
}

else if (LoadingFlag==4.) {
                          // dsig11dt,dsig22dt,dsig33dt given

PorousStressRt->ve[0] = PrescribedValue1;
PorousStressRt->ve[1] = PrescribedValue2;
PorousStressRt->ve[2] = PrescribedValue3;

mv_mlt(Kdot,PorousStressRt,StrainRate);

```

```

    }

    PorousStress = v_get(6);
    sv_mlt(timestep,PorousStressRt,PorousStress);

    strain = v_get(6);
    sv_mlt(timestep,StrainRate,strain);

    f_end = VoidFractionUpdate(StrainRate,f_start,timestep);
    new_axis_lengths = AxisUpdate(StrIntensity,StrainRate,
                                timestep,AxisLengtha_start,
                                AxisLengthb_start,
                                AxisLengthc_start,f_start,
                                f_end,MajorAxis,VoidType);
}

else { /* LoadingFlag=5 therefore use the pseudo-inverse
        calculations */

    // Assign value to MajorAxis

    MAX = fabs(PrescribedValue1);
    MajorAxis = 1.;

    if (MAX < fabs(PrescribedValue2)) {

        MAX = fabs(PrescribedValue2);
        MajorAxis = 2.;

    }

    if (MAX < fabs(PrescribedValue3)); {

        MAX = fabs(PrescribedValue3);
        MajorAxis = 3.;

    }

    /* Procedure for assigning values to StrainRate if using
    the DeformationGradient

    strain = v_get(6);
    Strain (Hencky,DeformationGradient,strain,
           Mapping,&Det);

```

```

StrainRate = v_get(6);
sv_mlt ((1./timestep),strain,StrainRate);    */

// Procedure for assigning values to StrainRate during
testing ie. defining terms directly using PrescribedValue1,
PrescribedValue2 and PrescribedValue3

StrainRate = v_get(6);
StrainRate->ve[0] = PrescribedValue1;
StrainRate->ve[1] = PrescribedValue2;
StrainRate->ve[2] = PrescribedValue3;

strain = v_get(6);
sv_mlt (timestep,StrainRate,strain);

Eshelby = EshelbyTensor(poissonRatio,AxisLengtha_start,
                        AxisLengthb_start,MajorAxis);
InvStrIntensity = InvStrIntensityTensor(Eshelby,f_start);
StrIntensity = FormInverseMatrix(InvStrIntensity);

B = B_Matrix(w_start,f_start,yieldStress,MajorAxis,
             VoidType);
H = HardeningRate(StressStart,f_start,w_start,MajorAxis,
                  yieldStress,StrIntensity,B,VoidType);
Kdot = FormDynStiff(StressStart,B,H);

PseudoInverse = CalcPseudoInverse(Kdot);

PorousStressRt = v_get(6);
PorousStress = v_get(6);
mv_mlt (PseudoInverse,StrainRate,PorousStressRt);
sv_mlt (timestep,PorousStressRt,PorousStress);

/* Since the prescribed strain rate values do not
conform to the form predicted by the PCZ model they tend
volume fraction and semi-axis lengths. To try and remedy
this situation it is proposed that the stress rate values
predicted using the pseudo-inverse calculations
(PorousStressRt) be used with Kdot to produce strain rate
values (PseudoStrRt) which conform to the PCZ model
and hence will produce better approximations of the
evolution of the internal variables */

PseudoStrRt = v_get(6);
mv_mlt (Kdot,PorousStressRt,PseudoStrRt);

```

```

f_end = VoidFractionUpdate(PseudoStrRt,f_start,
                           timestep);

new_axis_lengths = AxisUpdate(StrIntensity,PseudoStrRt,
                              timestep,AxisLengtha_start,
                              AxisLengthb_start,
                              AxisLengthc_start,f_start,
                              f_end,MajorAxis,VoidType);

m_free(Mapping);
m_free(PseudoInverse);
v_free(PseudoStrRt);
}

elasticity = ElasticityTensor(youngsModulus,poissonRatio);

ElasticStress = v_get(6);
mv_mlt(elasticity,strain,ElasticStress);

incStress = v_get(6);
v_copy(PorousStress,incStress); /* Here incremental stress only
                                consists of the porous stress for
                                testing purposes */

// v_add(PorousStress,ElasticStress,incStress);

finalStress = v_get(6);
v_add(StressStart,incStress,finalStress);

D = Linearization(incStress,strain,youngsModulus,poissonRatio,
                  elasticity,stressType);

*ResultStress = v_copy(finalStress,VNULL);
*ResultD = m_copy(D,MNULL);

*ResultIntVariables = new double[5];
(*ResultIntVariables)[0] = f_end;
(*ResultIntVariables)[1] = new_axis_lengths->ve[0];
(*ResultIntVariables)[2] = new_axis_lengths->ve[1];
(*ResultIntVariables)[3] = new_axis_lengths->ve[2];
(*ResultIntVariables)[4] = H/youngsModulus;

m_free(Mapping);
m_free(StrIntensity);

```

```

        m_free(InvStrIntensity);
        m_free(Eshelby);
        m_free(D);
        m_free(elasticity);
        m_free(Kdot);
        m_free(B);
        v_free(finalStress);
        v_free(incStress);
        v_free(PorousStressRt);
        v_free(PorousStress);
        v_free(ElasticStress);
        v_free(StrainRate);
        v_free(strain);
        v_free(new_axis_lengths);
    }
}

else { /* Invalid flags have been assigned */

    printf("\nAN ERROR HAS OCCURRED IN ASSIGNING
    VALUES TO FLAGS: SEE ABOVE OUTPUT STATEMENT\n");

    finalStress = v_get(6);
    *ResultStress = v_copy(finalStress,VNULL);
    D = m_get(6,6);
    *ResultD = m_copy(D,MNULL);
    *ResultIntVariables = new double[4];
    (*ResultIntVariables)[0] = 0;
    (*ResultIntVariables)[1] = 0;
    (*ResultIntVariables)[2] = 0;
    (*ResultIntVariables)[3] = 0;
    m_free(D);
    v_free(finalStress);
}
}

```