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1 **2D Distinct Element Modeling of the Structure and Growth of Normal Faults in**
2 **Multilayer Sequences. Part 1: Model Calibration, Boundary Conditions and Selected**
3 **Results**

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8 **Abstract**

9 The Distinct Element Method (DEM) is used for modeling the growth of normal faults in
10 layered sequences. The models consist of circular particles that can be bonded together with
11 breakable cement. Size effects of the model mechanical properties were studied for a constant
12 average particle size and various sample widths. The study revealed that the bulk strength of
13 the model material decreases with increasing sample size. Consequently numerical lab tests
14 and the associated construction of failure envelopes were performed for the specific layer
15 width to particle diameter ratios used in the multilayer models. The normal faulting models
16 are comprised of strong layers (bonded particles) and weak layers (non-bonded particles) that
17 are deformed in response to movement on a predefined fault at the base of the sequence. The
18 modeling reproduces many of the geometries observed in natural faults, including: (i)
19 changes in fault dip due to different modes of failure in the strong and weak layers, (ii) fault
20 bifurcation (splaying), (iii) the flexure of strong layers and the rotation of associated blocks to
21 form normal drag, and (iv) the progressive linkage of fault segments. The model fault zone
22 geometries and their growth are compared to natural faults from Kilve foreshore (Somerset,
23 UK). Both the model and natural faults provide support for the well-known general trend that
24 fault zone width increases with increasing displacement.

1 Introduction

Normal faults are not simple planar structures but zones containing numerous anastomosing fault strands, fault segments and associated structures e.g. fracturing and bed rotation [Wallace and Morris, 1986; Cox and Scholz, 1988]. Fault zone complexity arises from two main processes, the linkage of fault segments and the removal of fault surface asperities [Childs *et al.*, 1996b]. The formation of segmented faults and fault surface asperities has previously been attributed to the bifurcation and refraction of the fault surface as it propagates through a layered sequence [e.g., Walsh *et al.*, 2003]. The principal limitations of previous work are that they provide only a conceptual, rather than a mechanistic basis for the structure and growth of fault zones; here we present a suite of Distinct Element Method (DEM) models that investigate the mechanics of fault zone evolution within multilayered sequences.

Over the last decade the DEM has become an important tool for modeling the growth and interaction of faults and fractures. The DEM is capable of modeling the growth of discontinuities, such as faults, without the limitations of continuum mechanics. The elements interact with each other via a force displacement law and can be of arbitrary shape, rectangular blocks and spheres being the most common ones. Applications range from mining and engineering [Theuerkauf *et al.*, 2003], seismicity [Toomey and Bean, 2000] to soil and rock mechanics [Hart, 2003]. Recently the DEM has also been used to model tectonic processes such as the formation of shear zones and deformation bands [Antonellini and Pollard, 1995; Mora and Place, 1998; Morgan and Boettcher, 1999], displacement transfer and linkage of pre-existing faults [Walsh *et al.*, 2001; Imber *et al.*, 2004], failure in brittle rock on a small scale [Donzé *et al.*, 1994; Hazzard *et al.*, 2000] and on a large scale

[Saltzer and Pollard, 1992; Burbidge and Braun, 2002; Strayer and Suppe, 2002; Finch et al., 2003, 2004; Strayer et al., 2002, 2004; Cardozo et al., 2005; Seyferth and Henk, 2006].

The aim of this paper is to describe an application of the 2D DEM to modeling the development of the internal structure of normal fault zones, and to demonstrate that this application replicates, both qualitatively and semi-quantitatively, the internal structure of real faults. The paper firstly describes the DEM approach to modeling rock deformation, concentrating on two key aspects which need to be considered when designing and interpreting models of outcrop-scale geologic structures; these are, the effect of resolution, or numbers of particles, on rheological properties and the variation between different realizations of the same model. The paper then compares DEM models of normal fault development in a multilayer with a high strength contrast with natural fault zones in a similar (limestone/shale) sequence from Kilve foreshore, Somerset, UK [Peacock and Zhang, 1993; Peacock and Sanderson, 1994]. The observed similarity between the natural and model fault zones provides the basis for exploring the impact of confining pressure and strength contrast on the geometry and mechanics of normal faults in layered sequences presented in a companion paper (Schöpfer et al., Part 2).

2 Principles of Distinct Element Method (DEM)

2.1 Background

The Distinct Element Method (DEM) for circular particles was introduced by Cundall and Strack [1979]. The DEM implements the discrete-element method, which is a broader class of methods that allow finite displacements and rotations of discrete bodies [Cundall and Hart, 1992]. The commercially available Particle Flow Code in two dimensions (PFC2D, Itasca Consulting Group, [1999]) models the movement and interaction of circular particles

using the DEM. The particles are treated as rigid discs and are allowed to overlap at particle-particle and particle-wall contacts. Walls are rigid boundaries, that allow the user to define boundary conditions, e.g. constant velocity or stress, but are not accelerated due to interaction with particles. The amount of overlap is small compared to particle size and is proportional to the contact force. Both normal and shear forces arise at contacts. Slip can occur at particle-particle and particle-wall contacts when a critical shear force, which is defined by the contact friction coefficient, is exceeded. Particles and walls are defined by (i) normal and shear stiffness, k_n and k_s , (i.e. contact Young's and shear modulus) and (ii) contact friction coefficient, μ_c .

Bonds can exist between particles, but not between particles and walls. In the present study a linear (elastic) force-displacement contact model is used and particles are either non-bonded or bonded with a linear elastic material (parallel bond model). A parallel bond is defined by (i) normal and shear stiffness, $\bar{k}_n$ and $\bar{k}_s$, (ii) tensile and shear strength, $\bar{\sigma}_c$ and $\bar{\tau}_c$ (iii) and its bond-width multiplier, $\bar{\lambda}$. A bond-width multiplier of 1 completely fills the throat between two particles, whereas if the multiplier approaches zero the material behaves like a granular material. If either the tensile or shear strength (in stress units) is exceeded the bond will break and is removed from the system. In contrast to the often-used contact bond [e.g., Hazzard *et al.*, 2000; Strayer and Suppe, 2002; Finch *et al.*, 2003, 2004], which does not have stiffness and width and can only transmit forces, a parallel bond can transmit both forces and moments [Potyondy and Cundall, 2004]. Additionally a parallel bond allows slip prior to failure, whereas a contact bond inhibits slip. Most importantly, Wang *et al.* [2006], who implemented the parallel bond model using finite rotations rather than relative rotations and tangential motion as in PFC, have shown that a parallel bonded material better reproduces rheological properties of rock than a contact bonded material. The

failure of a parallel bond causes a decrease in stiffness of the system, which leads to a larger load on adjacent bonds than contact bond failure (pers. comm. Potyondy, 2003). New bonds, simulating annealing, are not created in this study.

The particles obey Newtonian dynamics (law of motion) and a force-displacement law is applied to each contact. The calculation cycle in PFC is as follows: (i) update contacts from known particle and wall positions, (ii) apply the force-displacement law to each contact to update contact forces, and (iii) apply the law of motion to each particle to update its velocity. This calculation cycle is performed using a time-stepping algorithm. The time step at each calculation is automatically chosen to be so small that during a single time step disturbances of any particle cannot propagate further than to its immediate neighbors. For a more detailed treatment on this numerical method the reader is referred to *Cundall and Hart* [1992], *Hazzard et al.* [2000], *Potyondy and Cundall* [2004, and references therein].

2.2 *Micro- and Macroproperty relations*

Model microproperties, such as particle stiffness, contact friction, bond stiffness and bond strength determine the rheological macroproperties of a model material. The generation of a model material involves determining the combination of microproperties, which reproduce the desired macroproperties, by calibrating the results of synthetic mechanical test procedures with those of real rocks (a good example is provided by *Kulatilake et al.* [2001]). Standard mechanical tests are: (i) Direct tension tests, (ii) Brazilian disk test (an indirect measure of tensile strength), (iii) unconfined, and (iv) confined compression tests. These tests are necessary to ensure that the bulk properties, such as Young's modulus, Poisson's ratio, tensile and compressive strength replicate those of the rocks to be modeled. All of these tests have been used here to define the macroproperties of the model materials.

Previous results, both analytical and numerical, have shown that the elastic macroproperties are, for a given particle size distribution, controlled by the contact normal and shear stiffness [Bathurst and Rothenburg, 1988; Rothenburg et al., 1991; Bathurst and Rothenburg, 1992; Fakhimi et al., 2002]. These studies have shown that Young's modulus increases linearly with increasing contact normal stiffness. Additionally Young's modulus decreases, whereas Poisson's ratio increases nonlinearly with increasing ratio of contact normal to shear stiffness, k_n/k_s . In summary, for modeling rock, the ratio of contact normal to shear stiffness should always be greater than 1 and, dependent on particle packing, realistic Poisson's ratios are obtained for $2 < k_n/k_s < 3$ (notice that incompressibility, $\nu = 0.5$, can not be obtained in fully bonded PFC models). Finally analytical and numerical modeling has shown that the elastic properties depend on particle packing (e.g. average coordination number; Bathurst and Rothenburg, [1988]), but are independent of particle size/resolution.

The bulk strength of a parallel bonded particle model with a random particle distribution and normally distributed bond strength can not be estimated analytically, since both the irregularity of the assemblage and stress concentrations that arise during bond breakage will affect the strength. Potyondy and Cundall [2004], however, proposed the following relationship:

$$K_{Ic} = \beta T' \sqrt{\pi \alpha r} , \quad (1)$$

where K_{Ic} is the Mode I fracture toughness, T' is the true tensile strength of the bonded particle model (i.e. the strength without stress concentrations), r is the particle radius and α (≥ 1) and β (< 1) are non-dimensional factors that account for the heterogeneous nature of the assembly and the weakening of the bending moments, respectively. Although equation (1)

does not predict the bulk strength of a bonded particle model, it reveals that fracture toughness and strength are dependent on particle size, which is therefore not a free parameter that determines model resolution. *Potyondy and Cundall* [2004] have additionally shown that bonded particle models are expected to have the same bulk tensile strength if the average number of particles across the width of the sample is held constant. This interdependence between particle size and sample size is crucial for the calibration process, since not only strength but also macroproperty variability is greatly affected by model resolution. Hence some of our modeling results that highlight this strength/size relation are presented below.

A list and description of the microproperties used throughout this study is given in Table 1. These properties were chosen (mainly by trial and error) because they provide macroproperties (Young's modulus, Poisson's ratio, unconfined compressive strength) and stress-strain response (e.g. figure 4 in *Schöpfer et al.*, [2006]) similar to sedimentary rocks (sandstone, limestone, shale) as discussed below.

3 Model Material Calibration

3.1 Specimen Generation and Testing Procedures

In this study the PFC2D model generation procedure and the biaxial and Brazilian disc testing environment described in Appendix A in *Potyondy and Cundall* [2004] are used. We use cylindrical particles with a uniform size distribution and unit thickness. For the biaxial compression tests the loading frame is rectangular with a height to width ratio of 2 (note that the bulk strength of bonded particles also depends on the width to height ratio; [*Place et al.*, 2002]). For the Brazilian tests the rectangular specimens are trimmed to a disc (Fig. 1).

In the case of biaxial tests the top and basal boundary move with constant velocity towards each other, while the stress acting on the lateral boundaries is held constant using a

stress servomechanism. During the tests the stress acting on the boundaries, the boundary positions and - for bonded materials - the location and timing of bond breakage events are monitored. Since the thickness of the cylindrical particles is unity the axial stress is simply the average force acting on the plates per incremental sample width. Brazilian disc tests were performed on bonded materials by moving the lateral plates towards each other. In a 2D disc sample with unit thickness the Brazilian (tensile) strength is the average force acting on the plates per half disc circumferences at failure.

To fully characterize the strength of the bonded model materials within the tensile field ($\sigma_3 < 0$), dog-bone shaped samples, trimmed from rectangular specimens, were tested at various confining pressures. The central width of the samples was 1m, i.e. the thickness of the strong layers in the multilayer faulting models (see below). A force equal to particle diameter times desired stress was applied to particles located at the lateral edges of the sample. The upper and lower straight-sided parts of the sample were pulled until failure occurred. The state of stress within the central portion was measured using a measurement circle with a diameter of 1m, containing on average 92 particles. Within this measurement circle, the average stress is calculated using the contact forces and the volume occupied by the particles within a circular region [Potyondy and Cundall, 2004]. Only samples where the measurement circle straddles the macroscopic fracture were used for determining the failure envelope of the material.

3.2 *Impact of Sample Size on Macroproperties*

Potyondy [2002] and Potyondy and Cundall [2004] emphasized that particle size/resolution is not a free parameter in PFC. A series of models were run with the same microproperties as the strongest (bonded) and the weakest (non-bonded) material tested in this study (Table 1)

for variable sample width of 1, 2, 3, 4 and 5m (Figure 1). The average particle diameter to sample width ratios are therefore 11.7, 21.3, 32.0, 43.7 and 53.3. The bonded material was tested using Brazilian tests (tensile strength) and unconfined compression tests, whereas the non-bonded material was tested using biaxial tests at a confining pressure of 25 MPa. The smallest samples had a width equal to the thickness of the bonded layers in our multilayer faulting models, i.e. 1m. For each sample size, 30 model realizations with different particle arrangements but identical microproperties were tested.

Figure 2 summarizes the results obtained from the sample size sensitivity study. In the case of the bonded material, the tensile strength, the unconfined compressive strength and the strain at failure decrease with increasing sample size, i.e. the material becomes weaker (Figure 2a – c). A similar non-linear relationship is obtained when the sample size is held constant and the particle size is varied, i.e. the tensile strength decreases with decreasing particle size (table 3 in *Potyondy and Cundall [2004]*). Interestingly, similar results have been obtained for natural rocks [e.g., *Jaeger and Cook, 1976; Scholz, 2002; Paterson and Wong, 2005*]. In our PFC2D models the tensile strength, however, decreases more rapidly than the unconfined compressive strength with increasing sample size. As a consequence the ratio of unconfined compressive strength to tensile strength increases with increasing sample size (Figure 2d). The ratio of compressive to tensile strength is, at 3 - 4.5, lower than for natural rocks (generally between 10 and 20). This is probably due to the smooth nature of the particles. *Fakhimi [2004]* has shown, that slightly overlapped circular particles, which are effectively particles with irregular contacts, can increase the compressive to tensile strength ratio.

Young's Modulus and Poisson's ratio are independent of sample size for samples $\geq$ 2m (Figure 2e and f, respectively). The confined (25 MPa) compressive strength of the non-

bonded material exhibits weak sample size dependence for sample widths of less than 3 m (Figure 2g).

The coefficients of variations for all measured properties decrease with increasing sample size (Figure 2h), though the tensile strength exhibits a greater variation than the other parameters. An important result of the sample size sensitivity analysis is the variability of the macroproperties when microproperties are held constant. This variability arises from the different particle and bond arrangements and has important consequences for the variability of model fault zone structure as described below.

There are two important length scales in DEM models, the sample size and particle size. Models with the same particle to sample size ratios (i.e. resolutions) will yield similar results. In this section we therefore could have obtained very similar results with a fixed sample size and variable particle size. For some purposes this means that it is not necessary to define a real world length scale, but for geological applications this will rarely be true as there are many scale dependent geological parameters, e.g. gravity, crustal thickness and the spacing between joints. The fault zone models discussed here are defined for a sequence of several individual, homogeneous beds with the properties of intact rock. Homogenous, i.e. non-bedded or non-jointed, layers of sediments (limestone, sandstone, shale) are rarely much thicker than a few metres. At larger scales, rock mass relations, which incorporate the presence of fractures, need to be considered [e.g. *Schultz*, 1996]. Our definition of homogeneous beds with material properties comparable to those of intact rock therefore implies a real world length scale.

3.3 *Properties of Materials Comprising the Multilayer Models*

In this section the properties of the materials used in the multilayer faulting models are described in detail. As highlighted in the previous section, mechanical properties are sample size dependent so that the properties of the multilayer materials are defined using test sample widths equal to the thickness of the beds in the multilayers, i.e. 1m. Multiple realizations of tests were carried out to investigate the variability in mechanical properties which can be expected to occur at the scale of the bedding.

The macroscopic behavior of four different bonded materials, with average tensile bond strengths of 300, 250, 200 and 150 MPa (microproperties are given in Table 1), were determined using dog-bone shaped sample tests at various confining pressure, unconfined and confined biaxial tests. The bond strengths are normally distributed with a standard deviation of 25 MPa (CV of 1/12 and 1/6 for the tensile and shear strength distributions, respectively) and a two standard deviation cut-off. Particles and cement (i.e. bonds) have the same elastic properties. The number of floating particles (particles with no bonds) is 4%; these floating particles were generated in order to reproduce the model material in the multilayer models (see below). One non-bonded material with the same particle elastic microproperties as the bonded materials and a contact friction coefficient of 0.5 was tested using confined biaxial tests (Table 1).

The results of the tests on the 1m wide dog-bone shaped samples are shown in Figure 3. For each material the least-square best-fit Coulomb-Mohr failure envelope with tension cut-off [Paul, 1961] was determined. The Coulomb-Mohr criterion expressed using the principal stresses can be written as [Jaeger and Cook, 1976]

$$\sigma_1 = \sigma_{uc} + q\sigma_3, \quad (2a)$$

where σ_{uc} is the unconfined compressive strength and

$$q = [(\mu^2 + 1)^{1/2} + \mu]^2 = \tan^2(\pi/4 + \varphi/2), \quad (2b)$$

where μ is the coefficient of internal friction equivalent to $\tan\varphi$. The intercept of this straight-line failure envelope with the tension cut-off is at:

$$\sigma_1 = \sigma_{uc} \left(1 - \frac{(\sqrt{\mu^2 + 1} + \mu)^2}{R} \right), \quad (3)$$

where R is the ratio of unconfined compressive strength to tensile strength (positive value).

The best-fit unconfined compressive strength values obtained are up to 15% greater than those obtained from the unconfined compression tests, reflecting the different boundary conditions (wall vs. particle boundary conditions), different loading methods and/or different measurement techniques (forces on walls vs. measurement circles).

The results of the 1m wide biaxial tests are summarized in Figure 4 and the mean values of the material parameters are additionally given in Table 2. Cumulative frequencies of tensile strengths obtained from the unconfined dog-bone tests are shown in Figure 4d. The properties of each of the bonded materials were determined from 30 unconfined and 30 confined ($P_c = 25$ MPa) biaxial tests. For each model pair (confined and unconfined) the friction angle and the cohesion were obtained. The friction angle for the non-bonded (i.e. cohesionless) material ($N = 30$) was obtained from biaxial tests at a confining pressure of 25 MPa.

The material properties obtained from the biaxial tests are comparable to those of limestone [e.g., *Al-Shayea*, 2004; *Tsiambaos and Sabatakakis*, 2004]. If the average strengths given in Table 2 are downscaled to samples with a diameter of 50mm using the scaling relationship given by *Hoek and Brown* [1997] the unconfined compressive strengths of the four bonded materials range from ca. 220 MPa to 110 MPa, strengths that are typical of intact sedimentary rocks. *Van de Steen et al.* [2002] investigated the tensile strength of crinoidal limestone using Brazilian tests with a diameter of 40mm. Their strongest samples had a tensile strength of 22 MPa. The upscaled strength for a 1m thick limestone bed can be obtained using a power law relationship between strength and sample size with an exponent of 1/6, which has been shown to fit experimental data for the tensile strength of concrete and sandstone [*van Vliet and van Mier*, 2000]. It follows that the theoretical strength of a 1m thick crinoidal limestone bed is approximately 13 MPa, a value that is obtained only for the weakest bonded material (Figure 4d). The tensile strength for the other bonded model materials is thus very high and up to a factor of 2 higher than for the natural samples described above. This reflects the fact that the ratio of unconfined compressive strength to tensile strength in DEM models presented with smooth, circular particles is lower than for natural rocks as mentioned in the previous section. The very high tensile strengths and the low UCS/T ratios of the model materials have the effect of transforming the failure mode transitions related to other materials (see figure 5 in Schöpfer et al., Part 2), but do not have a fundamental impact on the basic conclusions drawn from this study.

4 Fault Zone Modeling

In this section reproduction of the geometric features of faults in outcrop is attempted to demonstrate that the DEM microproperties can be calibrated, not only to mechanical test

results, but that the model material replicates the deformation of rock sequences and particular fault related structures. Examples of normal faults from Kilve foreshore, Somerset, UK, were selected for comparison with model faults.

4.1 *Fault Zone Geometry of Normal Faults, Kilve Foreshore, Somerset, UK*

Small-scale fault zones are exposed at Kilve foreshore on the southern margin of the Bristol Channel, UK [e.g., *Peacock and Sanderson, 1994; Glen et al., 2005*]. The faults cut a limestone-shale succession of Early Jurassic age, in which the shale units are generally thicker (from a few centimeters to >300 cm) than the intervening limestone beds (from a few centimeters to >50 cm). Normal faults of Late Jurassic to Early Cretaceous age formed during the development of the Bristol Channel Basin [*Chadwick, 1986*]. The depth of burial at the time of normal faulting is unknown, but vitrinite reflectance data suggest erosion of at least 1.5 km (and possibly as much as 3 km) due to Cretaceous/Tertiary inversion [*Cornford, 1986*]. Occasional bedding-parallel, partly calcite infilled cavities suggest that the shale layers were, at some stage during burial, overpressured. Normal faults contained in this high strength contrast sequence typically exhibit staircase geometry with steeply dipping faults within the strong limestone layers and shallow dipping faults within the weak shale layers (see antithetic fault cutting layer A and B in Figure 5b). Displacement along these refracting faults leads to the development of pull-aparts within the layers, which are typically infilled with ferrous calcite [*Davison, 1995*], although shale infill occurs occasionally [*Peacock and Sanderson, 1994*]. Some pull-aparts are infilled with fibrous calcite exhibiting initial wall perpendicular growth, followed by oblique fiber growth. This mineral infill is interpreted to record the growth history of faults within the limestone bed, i.e. initial extension (Mode I) fracturing followed by dip-slip movement. Mode I fractures occur on either side of fault

zones and are interpreted to represent zones of precursor fracturing, referred to hereafter as the 'fracture zone'. Fault surface asperities, arising both from the refraction of the fault surface through the multilayer and from the segmentation and bifurcation of the fault surface, appear to be removed with increasing displacement and sheared-off blocks of limestone are rotated, fractured and incorporated into the fault zone (Figure 5a). These rigid limestone blocks float in a ductile shale matrix. Space problems that arise due to geometrical complexities within the fault zone are typically accommodated by vertical and/or lateral flow of the shale (a decrease in shale thickness of >50% within the fault zone is not exceptional; see for example the difference in the thickness of the shale bed between layer A and B across the fault strand to the right hand side of the ruler in Figure 5a). The fault zones, therefore, accommodate the total displacement typically on two or more principal slip surfaces, between which the host rock sequence is variably deformed.

In order to quantify fault zone geometry and its dependency on throw, we measured fault zone width and total throw for 67 well-exposed fault zones. Profiles were measured across limestone bed platforms perpendicular to the average strike of the fault zone and parallel to bedding. For measurement purposes, fault zones were defined as zones comprising one or more kinematically related slip surfaces i.e. slip surfaces which are linked or demonstrate evidence of displacement transfer. Fault zone widths were measured as the distance between the outermost synthetic slip surfaces with visible shear displacement. Throw values include the net throw on all slip surfaces, together with offset accommodated by both normal drag and the rotation of fault bound blocks. Throw measurement errors are estimated to be in the range of a few millimetres and are mainly due to weathering and the hummocky nature of some beds.

The study of *Peacock and Zhang* [1993] is, to our knowledge, the only previous attempt to numerically model the evolution of fault zones similar to those exposed at Kilve foreshore. They used the DEM software UDEC, which is typically used for modeling faulted and jointed rock volumes. The fault geometries (extensional and contractional oversteps) in their models were, however, predefined and were not a direct response to mechanical layering. This study is the first attempt to model the initiation and growth of faults exposed at Kilve and similar normal faults contained in high strength contrast sequences.

4.2 *Multilayer Model Boundary Conditions*

Multilayer models are created using the specimen generation procedure described in section 3.1; models are 15 m wide, 13 m high and consist of >23,000 particles. Layering is introduced by assigning particles to three different groups, strong layers, weak layers or the top layer. The top layer is 3 m thick and its primary function is to confine the model. The model is confined by applying a force equal to particle diameter times desired stress to particles at the surface of the model; these particles are found using a mesh based searching algorithm. After model confinement, bonds are installed between particles comprising the strong layers, which are in this study always 1m thick and interbedded with 1.5 m thick weak, i.e. non-bonded, layers. Bonds are installed after confinement because if they were installed before confinement fracture boudinage would develop. Although bonding after confinement introduces a small proportion of floating particles (ca. 4%) within the bonded layers, this has no significant impact on our modeling results.

Localization of a single through-going fault is achieved by introducing a pre-cut 'fault' at the base of the multilayer sequence. The dip of the basement fault is 60° and the L-shaped wall on the hangingwall side of the pre-cut fault moves downward with constant

velocity (Figure 6). During model runs the stress at the base of the model and the location and timing of bond failure were recorded. The models were saved at 0.5m throw intervals, up to a final throw of 2-3 m.

5 Normal Faulting Results

In this section, selected results from the multilayer faulting experiments are presented and structures associated with faults at Kilve are compared with equivalent structures in the DEM models. A more comprehensive description of the modeling results and an analysis of the sensitivity of fault zone structure to layer strength and confining pressure are provided in the companion paper (Schöpfer et al., Part 2). Although some of the structural features of our models described below have been successfully modeled using analogue modeling [Horsfield, 1977; Withjack et al., 1990; Mandl, 2000] and continuum methods [e.g. Gudehus and Karcher, 2007], we are not aware of a modeling scheme, apart from that used in the present study, that is capable to reproduce all the structural elements described below.

5.1 Fault Growth and Geometry

To investigate the variability in fault zone structure, ten realizations of statistically identical models (table 1) were run using an average unconfined compressive strength of strong layers of 128.4 MPa and a constant confining pressure of approximately 46 MPa (a value corresponding to a 2km depth of faulting, assuming lithostatic conditions and an overburden density of 2500 kg m⁻³). Two representative models are shown in Figure 7 and together illustrate the capabilities of DEM in reproducing key features of the geometry of natural fault zones (Figure 5):

Fault nucleation: Initially a low amplitude (a few centimeters) monocline develops in the competent layers and extension (Mode I) fractures form due to horizontal tensile stress (Fig. 7). These early stages of fault nucleation, at throws of <10 cm are described in detail in Schöpfer *et al.* [2006] and Schöpfer *et al.*, Part 2. The hangingwall antithetic faults in the models shown in Figure 7a and b, which nucleate at a throw of 2 m on the main fault, illustrate the fault geometry typically observed at the nucleation stage in these high strength contrast models. The faults have a staircase geometry, dipping steeply in the strong layers and with shallower dips in the weak layers; their geometry is strikingly similar to the antithetic fault exposed at Kilve (Figure 5b). Further displacement on these irregular faults leads to the development of pull-aparts within the strong layers, for example where the antithetic fault offsets Bed A on Fig. 5b and in the model example, where the large antithetic fault in Fig. 7b at a throw of 3m offsets the second highest bed.

Normal drag: The flexure of layers adjacent to a fault is referred to as drag; where the sense of drag is the same as the sense of fault offset it is referred to as normal drag. Normal drag is a common feature in both Kilve and the models. The field example shown in Figure 5a (layer A and B) highlights that drag at Kilve occurs by the rotation of initially fractured blocks. The model fault zone in Figure 7b (especially at a throw of 1 and 1.5 m) exhibits the same drag geometry as seen at Kilve, and the different model stages illustrate the amplification of drag and the progressive rotation of wall rock blocks into the fault zone with increasing displacement.

Asperity removal: In the model shown in Figure 7a a single, convex upwards fault develops up to a throw of 0.5m. This irregularity in fault trace geometry represents an asperity which, with increasing throw, is progressively by-passed by the formation of a second slip surface in the footwall. This new slip surface is itself locally convex upwards so that, at a throw of

2.0m, another fault develops in its footwall. The final geometry is a fault zone with stacked fault bound lenses that contain rotated blocks of the strong layers. Similar geometries, including stacked lenses, are associated with the faults at Kilve (see lenses to right of the half-arrow in Figure 5a and where layer C is offset in Figure 5b), and may, by analogy with the models, have been formed by asperity removal.

Fault linkage: This process occurs when two segments of a fault array become linked to form a single through-going, though not necessarily planar, active fault. The different stages in fault linkage can be seen in the model shown in Figure 7b, where two overlapping fault segments bound a contractional overstep at a throw of 0.5m. This fault geometry cannot accommodate significant displacement and increasing displacement leads to the breaking up of the strong layers and squeeze flow of the weak ones within the fault zone. Linkage of the two segments leads to the formation of a concave up fault, which in turn leads to the formation of antithetic faults as described below.

Antithetic faults: Faults that dip in the opposite direction to the master fault develop frequently, both in nature (Figure 5b) and in the models (Figure 7). Although some of the antithetic model faults are clearly due to the model boundary conditions used, many antithetic faults appear to be structures that accommodate local irregularities of the master fault. For example the development of antithetic faulting due to movement on a concave upwards fault can be seen in the growth sequence shown in Figure 7b (convex upwards irregularities typically lead to asperity removal in the models as described above). Although the natural fault shown in Figure 5b exhibits antithetic faulting, its origin cannot be reconstructed due to the large throw on the main fault, though fault bound lenses that are located adjacent to the branch-point of the antithetic faults with the main slip surface suggest that this part of the fault was originally irregular and possibly concave upwards.

5.2 Fault Zone Width vs. Throw

To establish whether our modeled fault zones also reproduce quantitative aspects of the fault geometries observed at Kilve, we measured the widths of the model fault zones, in each strong layer in the 10 model realizations. The criteria used for measuring fault zone widths were the same as those used in collecting the Kilve data and described above. In some cases the measured fault throw is greater than that on the precut fault. This occurs where offset on antithetic faults outside the measured fault zone is balanced by an increase in throw on the main fault zone maintaining the constant net throw.

The fault zone width data from Kilve and from the PFC models are plotted on a log fault zone width versus log throw plot in Figure 8. Comparison between the two data sets shows that the ratio between fault zone thickness and throw is the same over the measured throw range of the model faults. Both datasets suggest a positive correlation between fault zone width (w) and throw (t) of the form

$$\log w = n \log t + c \quad (4)$$

where n is the power-law exponent (typically about 1) and c is the $\log w$ intercept; the relationship for the model data is not as well constrained due to the limited throw range. Best-fit relationships of the form given in Equation 4 were fitted to the datasets using reduced major axis regression lines (RMA), where the slope of the line is the ratio of the standard deviations of the two variables [e.g. *Davis*, 1986]. This type of analysis permits semi-quantitative comparison of natural and modelled fault zone data. The Kilve and PFC data define similar positive trends (with correlation coefficients of 0.69 and 0.55, respectively),

which, despite significant scatter, have very similar regression lines. The slopes (n in equation (4)) for the natural and modelled fault zone widths are both close to 1 (0.97 and 0.84, respectively; significant equivalency at a 0.01 level) and the constant c (equation (4)) is also within the same order of magnitude (0.34 and 0.14 for Kilve and PFC models, respectively). It appears therefore that our models replicate both the variability and the growth trend of natural fault zones (although, as expected, the variability in nature is greater than in our models) suggesting that the processes which cause fault zone widening in the model faults (asperity bifurcation, fault linkage) are also likely to have occurred in the Kilve faults.

5.3 *Impact of Layer Strength on Fault Geometry*

A series of models with identical particle distributions was run at different confining pressures and strength of the strong layers (see Schöpfer et al., Part 2). Figure 9 shows the model results for the four different calibrated bonded model materials described above (average unconfined compressive strengths of 128.4, 106.4, 83.1 and 64.0 MPa) at a throw of 2 m and at a confining pressure of approximately 23 MPa (ca 1km depth for lithostatic conditions and an overburden density of 2500 kg m⁻³). The models highlight the control of layer strength on fault zone geometry and width. Although all four models exhibit many of the complexities described before, it appears that faults contained in high strength contrast sequences are more complex and also wider. A complete understanding of why strength controls fault geometry requires a mechanical analysis that focuses on both the stress and strain at the onset of fault, which is provided in the companion paper (Schöpfer et al., Part 2).

6 Discussion

The Distinct Element Method (DEM, as implemented in PFC2D) is a relatively new tool for modeling tectonic processes. Unlike in continuum methods, where the bulk properties and the macroresponse of the material are defined using constitutive equations, modeling using the DEM involves model calibration in order to establish the macroproperties of the model material. The models demonstrate that fault zone growth and geometry depend on the deformation conditions, the mechanical stratigraphy and random flaws. The model results in this paper are, however, presented in a qualitative, rather than quantitative, way. A more thorough presentation of the relationships between fault zone geometry and deformation conditions and the mechanical stratigraphy is given in the companion paper (Schöpfer et al., Part 2).

It is well known from rock mechanics that the bulk strength of rocks decreases with increasing sample size [Jaeger and Cook, 1976; Scholz, 2000; Paterson and Wong, 2005]. PFC2D shows similar size effects (Figure 2). Tensile strength, unconfined compressive strength and strain at failure decrease with increasing sample size, i.e. the model material becomes weaker with increasing sample size. Similar effects have previously been obtained if sample size is held constant and particle size is varied [Potyondy and Cundall, 2004]. Therefore scale-effects have to be considered if bonded particles are used. Interestingly the ratio of unconfined compressive strength to Brazilian strength increases with increasing sample size, which is due to the different scale dependence of compressive and tensile strength (Figure 2). This probably reflects the fact that the different types of macrofractures developed in the Brazilian and biaxial test environment (tensile failure vs. extension fracturing and faulting) have different scale sensitivity. Modeling results show that whilst the variability of bulk properties decreases with increasing sample size, the variability in tensile

strength is twice as high as the variability in unconfined compressive strength. This suggests that tensile macrofracturing in Brazilian tests is more sensitive to particle packing and bond arrangement than axial splitting and shear fracture in biaxial tests. This has important consequences for interpretations of the variability of modeled structures.

Four different bonded materials and one non-bonded material were used for modeling the growth of normal faults in layered sequences. The bulk properties of the bonded materials are similar to strong, sedimentary rocks (e.g. limestone), i.e. Young's modulus of approximately 21 – 22 GPa, Poisson's ratio of 0.24 - 0.31, and unconfined compressive strengths in the order of 64 – 128 MPa. The tensile strength is approximately a third of the unconfined compressive strength (Table 2), which is higher than for natural rocks. Additionally the friction angle of the bonded materials is slightly too low, i.e. 27 - 29 degrees. The difficulties of obtaining realistic compressive to unconfined compressive strength to tensile strength ratios and friction angles using smooth, circular particles is discussed by *Fakhimi* [2004], who suggested a modified DEM that can improve on these shortcomings. *Boutt and McPherson* [2002] used unbreakable particle clusters and successfully increased the friction angle, but whether they could increase the ratio of compressive to tensile strength is unknown since the tensile strength was not investigated. *Potyondy and Cundall* [2004] suggested the use of breakable particle clusters and recommended future studies using this approach.

The weak layers are modeled using non-bonded particles. This model material has no cohesion and a friction angle of ca. 27 degrees. The stress strain curves (not shown) indicate ductile behavior (flow at steady-state stress) at all confining pressures, whereas natural mudrocks typically exhibit different stress-strain responses at different confining pressures [e.g., *Petley*, 1999]. However, the bulk rheology satisfactorily models the ductile behavior of

the shale observed in the field (e.g. squeeze flow within the fault zone, infilling of pull-aparts). In addition to the shortcomings discussed above, the DEM modeling approach in this study does not incorporate strain rate sensitivity and fluids.

Despite the simplifications discussed above, the DEM modeling reproduces many features associated with natural fault zones in multilayers, including extension (Mode I) fracturing, normal drag folding, fault plane refraction, bifurcation (i.e. splaying) and segmentation. The high strength contrast/low confining pressure models presented in this study suggest the following growth history, which is consistent with conceptual growth models for natural fault zones: (i) Initially extension (Mode I) fractures form within the strong layers due to horizontal tensile stress. Though the link with natural examples is clear, some natural fault zones exhibit higher extension fracture density (e.g. Figure 5a) than those observed in the DEM models, a feature that may be attributable to the operation of crack-seal and associated annealing in nature, neither of which have been incorporated in the DEM models. (ii) Increasing displacement leads to linkage of the initially vertically segmented extension fractures. The formation of extension fractures in the strong layers and linkage via shallower dipping faults in the weak ones occurs continuously, since the fault zone widens and new fault splays and segments form (e.g. asperity removal, Figure 7a). (iii) Fault zones typically exhibit more than one slip surface. The fault-bounded blocks rotate towards the hangingwall to form normal drag and space problems are accommodated mainly by lateral flow of the weak material. It is likely, that out-of plane lateral flow is an important mechanism in natural faults, but the models are restricted to in-plane deformation.

The analysis and modelling demonstrates the very significant variability of fault zone structure arising from the operation of a few principal processes, fault refraction, segmentation and asperity removal. Simple 2D numerical modelling, in which the only factor

that controls fault zone variability is the distribution of weaknesses (flaws), suggests that the prediction of one particular cross-sectional fault zone structure (fault overstep or bend, straight fault) within a known sequence is probably impossible (Figure 7). Nevertheless, this relatively new modelling technique may prove capable of estimating the probability and frequency of fault zone complexities, especially if modelling is performed in 3D.

7 Conclusions

- The macroresponse of bonded particle models is dependent on scale and resolution. The strength of the material decreases non-linearly with increasing model size, whereas the elastic parameters are independent of sample size for samples with a width greater than 20 particles
- Models consisting of smooth, circular particles typically have low (3-5) unconfined compressive strength to tensile strength ratios, which increase with increasing sample size, and low friction angles. Much larger models than presented here are expected to exhibit more realistic ratios of unconfined compressive strength to tensile strength.
- Two-dimensional DEM modeling using layers of bonded and non-bonded particles successfully reproduce many of the structures observed in natural fault zones exposed in limestone/shale sequences at Kilve foreshore, Somerset, UK. Aspects of faulting which have been modeled successfully include (i) changes in fault dip due to different modes of failure in the strong and weak layers, (ii) fault segmentation, (iii) the flexure of strong layers and the rotation of associated blocks to form normal drag and (iv) the progressive linkage of fault segments.

- Previous conceptual models suggest that fault zone complexity arises from two main processes, the linkage of fault segments and the removal of fault surface asperities. For the first time these processes have been reproduced in numerical models without predefined faults.
- Different model realizations of a single model (i.e. unchanged microproperty definition) yield a range of results, not only for mechanical tests but also for fault zone internal structure.
- At a constant confining pressure and strength contrast, fault zone geometries are sensitive to the initial distributions of flaws. The modeling suggests that it is impossible to predict exact fault zone geometries within a given sequence at a particular confining pressure, but that the modeling has potential for predicting fault zone variability and the frequency of occurrence of particular fault geometries.

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Figure Captions

Figure 1. Biaxial tests (a and b) and Brazilian disks (c) used for sample size sensitivity study (the largest samples are 5m wide). Microproperties are given in Table 1 (average tensile bond strength of bonded material 300 MPa). For each sample size the average macroproperties were obtained from 30 different particle assemblies. (a) Biaxial tests with non-bonded particles at a confining pressure of 25 MPa and an axial strain of 1%. Only particles exceeding the average particle rotation are shown (black = anticlockwise, grey = clockwise). Notice that an effective conjugate system of shear zones cannot develop in small samples and that the width of the shear zones is 5-10 particles. (b) Unconfined biaxial tests using bonded particles at a strain of 0.5% after failure has occurred. Black lines indicate broken bonds. Both shear failure and axial splitting occurs. (c) Brazilian disks after failure. Although tensile stress exists in the centre of the disc prior to failure [e.g., *Jaeger and Cook*, 1976], fractures propagate from the side towards the centre of the disc, which is common for materials with low unconfined compressive strength to tensile strength ratios [*Fairhurst*, 1964].

Figure 2. Relationships between sample size and macroproperties of model material (microproperties are given in Table 1; $\bar{\sigma}_c = 300$ MPa). Circles and squares denote tangent and secant elastic parameters in (e) and (f), respectively (different symbols are used in (h)). Best-fit curves of the form $y = (1+ax)/(b+cx)$ together with the best-fit parameters are given for the data in graphs (a) to (d). Bars denote one standard deviation ($N = 30$ for each sample size).

Figure 3. Model calibration results obtained from dog-bone shaped samples with a central width of 1m. The stress at failure was determined using a measurement circle with a width of 1m, located in the centre of the sample. The average tensile bond strengths, $\bar{\sigma}_c$, of the four materials are given in each graph and one of the tested samples is shown in the uppermost diagram. Other microproperties are given in Table 1; the model material contains 4% floating particles. The values given in each diagram are the least-square best-fit results. Probability curves (0.1, 0.5, 0.25, 0.75, 0.95 and 0.99) were determined by keeping the best-fit ratio of unconfined to tensile strength and the friction coefficient constant. Fractional probability values for each curve are calculated as the sum of the differences in σ_3 between the curve and each point to the right hand side of the curve, divided by the σ_3 difference for all points.

Figure 4. Cumulative frequency distributions obtained from 1m samples ($N = 30$). The tensile strength (d) was obtained from dog-bone shaped samples with a central width of 1m; all the other macroproperties were obtained from biaxial tests. The average values are provided in Table 2. Only the angle of internal friction (e) was obtained for the non-bonded material, since this material has no cohesion and deforms in a ductile manner.

Figure 5. Interpreted photographs of normal faults exposed at Kilve foreshore, Somerset, UK. (a) Fault zone located at Quantock's Head (ST 13571 44215). Notice splaying, rotation of fault bound blocks and their progressive incorporation into the fault zone. (b) Fault zone located east of Kilve Pill (ST 14927 44588). Notice antithetic fault exhibiting fault refraction, i.e. fault dip variations in different lithologies.

Figure 6. Model boundary conditions. PFC2D model consisting of >23,000 bonded (white) and non-bonded (grey) cylindrical particles. The blow-up of the model shows particles joined by bonds and illustrates the resolution of the models. Each particle represents a volume of rock, rather than individual grains.

Figure 7. Multilayer model result illustrating formation of fault bound lenses due to (a) asperity bifurcation and (b) linkage of overstepping fault segments. White and grey layers consist of bonded and non-bonded particles, respectively, and t = throw. Average unconfined compressive strength of the strong layers is 128 MPa and confining pressure is 46 MPa (equivalent to ca 2km depth for lithostatic conditions and an overburden density of 2500 kg m⁻³). Black lines are particle separations > 1 cm. The only difference between the two models is the initial particle and bond arrangement.

Figure 8. Log-log plot of fault zone width vs. throw. Solid and dashed lines are RMA regression lines of the Kilve and model data, respectively.

Figure 9. Multilayer model results indicating a decrease in fault zone complexity with decreasing strength contrast. White and grey layers consist of bonded and non-bonded particles, respectively, throw in all models is 2.0m and confining pressure is approximately 23 MPa. $\bar{\sigma}_c$ = average unconfined compressive strength (strength distributions are shown in Figure 4). Black lines are particle separations.

Table 1. PFC2D microproperties of materials comprising the multilayer models

Microparameter	Description	Bonded Particles	Non-bonded Particles
r_{min}, r_{max} , mm	lower and upper limit of particle radii (uniform distribution)	31.25, 62.50	31.25, 62.50
k_n , GPa	Young's modulus at contact	50	50
k_n / k_s	ratio of particle normal to shear stiffness	3	3
μ_c	particle friction coefficient	1.0	0.5
$\bar{k}_n$, GPa	Young's modulus of parallel bond	50	-
$\bar{k}_n / \bar{k}_s$	ratio of bond normal to shear stiffness	3	-
$\bar{\sigma}_c$, MPa	average normal bond strength (coefficient of variation of normal distribution is 1/12)	300, 250, 200 and 150	-
$\bar{\tau}_c$, MPa	average shear bond strength (coefficient of variation of normal distribution is 1/6)	150, 125, 100 and 75	-
$\bar{\lambda}$	bond width multiplier	0.5	-

Table 2. PFC2D macroproperties of strong layers in multilayer models. The mean properties and their standard deviations for 30 realisations are given.

$\bar{\sigma}_c$, MPa	E , GPa	ν	σ_{uc} , MPa	T , MPa	C_0 , MPa	φ , °
300	21.82 ± 1.53	0.31 ± 0.05	128.39 ± 16.07	43.78 ± 7.14	37.78 ± 7.32	29.44 ± 5.60
250	21.79 ± 1.55	0.29 ± 0.06	106.39 ± 12.92	36.43 ± 5.95	31.54 ± 5.48	28.93 ± 5.11
200	21.56 ± 1.54	0.26 ± 0.06	83.07 ± 11.75	29.11 ± 4.74	24.89 ± 4.95	28.53 ± 5.07
150	20.99 ± 1.52	0.24 ± 0.06	64.00 ± 7.96	21.85 ± 3.54	19.85 ± 3.08	26.52 ± 4.26

















