DEM simulation of normal faults in cohesive materials

Steffen Abe *, Heijn van Gent, Janos L. Urai

RWTH Aachen University, Geologie-Endogene Dynamik, Lochnerstrasse 4–20 52056 Aachen, Germany

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A B S T R A C T

We performed Discrete Element Method (DEM) simulations of the formation of normal faults in a brittle-cohesive material above a basement fault, focusing on the formation of open fractures and cavities in areas of low normal stress, i.e. near the surface of the model. The simulations produce a wide range of fundamental structures similar to those observed in nature and in analogue models. Comparisons with these sandbox experiments show that the fundamental structures generated are similar between the analogue and the numerical models. In a parameter study of the material properties and the model geometry, we have investigated the effect of these parameters far beyond what is possible in analogue models. Over a range of parameters we show that the evolving structural style is robust, i.e. all the models develop similar structures in a similar sequence. Results show a systematic dependence of some structural features, such as location and style of faults, on the simulation parameters. In particular we observe that the maximum depth of the open fractures varies linearly with the cohesion suggesting that we can predict the depth of open cavities formed by tensile failure in natural fault systems if the material properties are known.

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1. Introduction

The formation of open fractures is often observed in normal faulting of cohesive materials under low normal stress. These structures occur in settings where the rock is strong (i.e. has a high brittleness index) compared to the mean effective stress. This occurs close to the surface or at high pore pressure at depth. Examples have been described in the extensional faulting of basaltic sequences of Kilauea volcano by Holland et al. (2006) and in carbonate rocks by Ferril and Morris (2003). Angelier et al. (1997) describe dominant tensile fracturing in the upper few hundreds of meters of the crust in Icelandic basalts with a transition to shear or hybrid failure at greater depth. These observations are similar to those of Acocella et al. (2003) in the Ethiopian rift zone.

The internal structure, in particular with respect to the existence and possible connectivity of open fault segments of these fault zones is important because it will determine the permeability of the faults and thereby the fluid flow through them (Ferril and Morris, 2003; Gudmundson, 2000). However, the details of the subsurface structure of these fault zones is difficult to obtain in nature.

One method that can be used to investigate the internal structures of fault zones are analogue models, i.e. sandbox experiments. Work by Holland et al. (2006), Holland et al. (2011), Galland et al. (2003), Galland et al. (2006) and van Gent et al. (2010) using cohesive powder have shown that fault structures similar to the geological prototypes can be obtained in the laboratory where it is possible to a much greater extent to investigate their internal structures, in 2D and in 3D, over time. However, there are still some limitations to those experiments. Firstly there is a limited ability to vary the details of the mechanical properties of the material used in the sandbox in order to match the scaled geological parameters. Additionally, numerical simulations make it much easier to vary the model geometry.

Also, while the experiments are more accessible than geological fault systems, there still are data which are difficult to obtain, for example local forces and velocity fields during the deformation. Numerical simulations in contrast allow a wide range of material parameters and full access to all internal data of the model. An added advantage of the numerical simulations is the ability to perform ensemble simulations without much additional effort except for the computing time spent.

Due to the inherently discrete nature of the problem we have decided to employ the discrete element method (DEM) for a numerical study of the evolution of normal fault systems in a brittle-cohesive material. DEM simulations have been used before for the investigation of fault zone development by Seyferth and Henk (2006) and Schöpfer et al. (2007a, 2007b) although for situations where the confining stesses have been much higher than cohesion of the rock and therefore no open fractures occur. An additional key advantage of numerical models is that the easy repeatability and the possibility to vary material properties allow it to perform parameter space studies. In this work we will use a large number of DEM simulations to perform a parameter space study. The results show the sensitivity of the structural evolution of faults in the model to the material properties and different boundary conditions. e will compare the results of a “baseline” numerical model...
with the analogue models of Holland et al. (2006) in order to validate the simulation results.

2. Simulation method

We use the Discrete Element Method (DEM) (Cundall and Strack, 1979; Mora and Place, 1994; Place and Mora, 1999; Potyondy and Cundall, 2004). While there are some differences between the various implementations of the DEM idea, all of them share the common fundamental concept that the model consists of spherical particles interacting with nearest neighbors either by brittle-elastic “bonded” interactions or by repulsive-elastic and frictional “contact” interactions. From these interactions the forces and moments acting on each particle can be calculated and the particle movements are then computed from the interaction forces using Newton’s law. The particle–particle bonds representing the linked interactions can break irreversibly if a deformation threshold is exceeded.

The microscopic interaction parameters are chosen such that the macroscopic elastic and fracturing behavior of the model material closely resembles that of a linear elastic solid. We are using frictional-elastic contact forces for unbonded particles coming into contact. There the normal force is calculated using a linear elastic contact law and the tangential force is calculated using a Coulomb friction law as described by Cundall and Strack (1979). To calculate the interaction forces between particles which are in cohesive contact we are using the rotational particle bond formulation by Wang et al. (2006). In order to enable the simulation of sufficiently large models an implementation of the DEM for parallel computers, ESyS-Particle, based on the parallelisation approach by Abe et al. (2003), has been used. The software is available as open source at https://launchpad.net/esys-particle/.

3. Model description

3.1. Model setup

For the initial studies presented in this work a 2D model has been used because its lower computational cost did make it possible to run a large number of simulations in order to explore the behavior of the model in a larger part of the parameter space. The geometry of the simulation models is derived from the laboratory sandbox experiments performed by Holland et al. (2006) and van Gent et al. (2010). However, in order to reduce the computational cost of the model only one half of the symmetric sandbox is used in the numerical models (Fig. 1). In that respect our numerical setup is closer to the analogue model used by Holland et al. (2011). The angle of the inclined fault at bottom can be adjusted arbitrarily.

While the material parameters used in the model are taken from laboratory data, the model geometry and the amount and velocity of the movement along the basement fault are modified to minimize the computing time necessary. While the model height \( H \) in Fig. 1 is set to 15 cm to match the vertical dimension of one of the experimental setups used by Holland et al. (2006) the horizontal dimension \( L \) in Fig. 1 is chosen to be as small as possible while keeping the model edges far enough from the active region of the evolving fault zone to avoid any unrealistic influence. In the simulations presented here \( L = 2H \) is chosen. Because we are mainly interested in the early stages for the development of the fault zone, the final displacement along the basement fault is only 10% of the model height \( H \).

The model is internally using “Model units” requiring a conversion from “Real world units” during setup of the model and back into “Real world units” at the post-processing of the results. For details of the conversion see Place et al. (2001). Here we give the basic geometric parameters in Table 1 both in “Model units” and in “Real world units” but subsequently we will be using the converted “real” units only in the paper.

In the laboratory experiments by van Gent et al. (2010), the gypsum powder is deposited in the box by sieving it from a prescribed height above the box which is several times larger than the height of the box itself. While it would be technically possible to simulate this process within the Discrete Element Model, we have chosen a different approach in order to minimize the computational costs involved. We apply a two-stage setup process. In a first stage a densely packed random particle arrangement is generated using algorithm by Place et al. (2001). This method uses an insertion based algorithm in which, after an initial seeding phase, particles are inserted into the model space in such a way that they always exactly touch 3 other particles or “walls”. If it is not possible to insert additional particles within the chosen size range which fulfill this condition, the algorithm terminates. The advantage of this algorithm is that it provides a relatively fast way to generate dense, random particle packings. After the initial particle packing has been generated the particles are then placed in the simulated sandbox (see Fig. 1), initially without inter-particle bonds and therefore without cohesive forces, and let to settle under a purely gravitational load until the elastic and gravitational forces are in equilibrium and there is no more particle movement. After this equilibrium configuration has been reached, bonds are created between touching particles thereby changing the interactions between these particles from purely repulsive elastic to brittle-elastic, thereby introducing cohesion into the material. After this setup process has been completed the boundary plates in the right part of the model (see Fig. 1) are moved down along the pre-defined fault plane. After an initial linear acceleration phase the velocity of the fault movement is kept constant. The boundary conditions, defined by the interactions between the particles and the walls which form the sandbox, are such that the particles touching the walls can freely slip in a direction tangential to the wall and having elastic interaction with the wall in the direction normal to the wall.

One model parameter which has not been taken directly from the laboratory experiments is the velocity at which the fault is moved. In order to minimize the computational cost of the models a fault velocity of \( v = 5 \) mm/s is used. This is faster than the values used in the experiments, i.e. between 0.01 mm/s (Holland et al., 2006) and

<table>
<thead>
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<th>Parameter</th>
<th>Model units</th>
<th>Real units</th>
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<tbody>
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<td>Minimum particle radius</td>
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<td>0.2 mm</td>
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<tr>
<td>Maximum particle radius</td>
<td>1.0 mm</td>
<td>1.0 mm</td>
</tr>
<tr>
<td>Model height</td>
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<td>15 cm</td>
</tr>
<tr>
<td>Model width</td>
<td>300 cm</td>
<td>30 cm</td>
</tr>
<tr>
<td>Number of particles</td>
<td>$\approx 56,000$</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1. Schematic drawing of the geometry of the model.
0.0166 mm/s (van Gent et al., 2010) and the long term average fault movement rates inferred from geological observations (mm-
cm/year, i.e. $10^{-7} \ldots 10^{-6}$ mm/s). However, tests using different velocities in the range $v = 0.5 \ldots 20$ mm/s for the fault movements show that at the velocities used in the main simulations the evolution of the models does not significantly depend on the velocity of the fault movement.

3.2. Material calibration

The material used in the experiments of Holland et al. (2006) and van Gent et al. (2010), i.e. hemihydrate powder ($\text{CaSO}_4 \cdot 1/2 \text{H}_2\text{O}$), shows a complicated relation between the compaction and porosity state and the strength of the material. Our current model is not capable of reproducing this behavior exactly. van Gent et al. (2010) have matched the behavior of the hemihydrate powder used in their experiments to a failure envelope similar to a cam-clay model (Jones and Addis, 1986; Roscoe and Schofield, 1963) and show that the cohesion of the powder increases with burial depth. Our model material is closer to a conventional Mohr–Coulomb material where the cohesion is independent of the mean stress. Key differences are that the numerical model material does not undergo irreversible compaction under normal loading and that, for stresses below the failure threshold, cohesion and tensile strength in the numerical model material are independent of the stress path the material has experienced.

To calibrate our model parameters a set of shear failure tests at a range of confining pressures have been performed. Because the numerical model material does not show any significant consolidation (i.e. very little inelastic compaction) under compressive loading, only tests with a constant applied normal force have been performed, similar to the “normally consolidated” test of van Gent et al. (2010). The results of these tests (Fig. 2) show a mainly linear failure envelope with some curvature at low confining stresses, similar to those observed by Holland et al. (2006). The apparent cohesion obtained from the linear fit in Fig. 2(a) is $C = 160$ Pa, whereas the extrapolation of the curved failure envelope suggests a cohesion value closer to $C = 110$ Pa. The value of 160 Pa calculated from the linear fit is slightly lower than the obtained by linear extrapolation of the linear part of the failure envelope in the experiments by Holland et al. (2006) (200 Pa). However, the value obtained by extrapolating the nonlinear failure envelope, i.e. $C = 110$ Pa is higher than the values Holland et al. (2006) and van Gent et al. (2010) obtained directly from the nonlinear failure envelopes, i.e. 62 Pa (Holland et al., 2006) and 40 Pa (van Gent et al., 2010). In the following we will assume the cohesion value obtained from extrapolation of the envelope (i.e. 110 Pa) as the true cohesion value of our simulated material. The tensile strength $T$ of the material was calibrated using a simulation of a direct tension test. The strength obtained is $T \approx 41$ Pa which is well within the range measured by van Gent et al. (2010) (30–50 Pa, depending on the compaction and burial depth of the material). The coefficient of internal friction calculated from the linear fit to the failure envelope in Fig. 2(a) is $\mu = 0.542$, therefore the friction angle $\phi = \tan^{-1} \mu$ can be calculated at $\phi = 28.5^\circ$. This friction angle is slightly smaller than that reported by Holland et al. (2006) which is $\mu = 0.71$, resulting in a friction angle $\phi = 35.4^\circ$. The friction angle in our numerical model is closer to but still smaller than the one measured by van Gent et al. (2010) for normally consolidated hemihydrate powder who obtained $\mu = 0.61$ and therefore $\phi = 31.4^\circ$.

The calibrated material properties in Table 2 show that we have obtained a close match of the strength and friction angle between the numerical model material and the hemihydrate powder used by Holland et al. (2006) and van Gent et al. (2010). However, as has been shown by Schöpfer et al. (2009), it is not always possible to obtain the desired friction angle and ratio between tensile and compressive strength (or cohesion) in a DEM model. We did therefore chose to match the strength parameter we considered most important for the evolution of structures in our model, i.e. the tensile strength. While it might be argued that the differences in the material parameters, although relatively small, could still influence the outcome of the simulations it needs to be taken into account that even for numerical methods where the material parameters can be exactly specified differences between analogue experiments and numerical simulations and between different numerical approaches have been observed (see, for example, Buitser et al., 2006). In addition we note that our models do not reproduce the compaction (burial depth) dependent increase in $T$ as described by van Gent et al. (2010).

4. Results

4.1. Analogue model comparison

The main features of the evolving fault zone which have been observed in the simulation models are shown in Fig. 3. In order to determine the location and timing of any fracture event in the model we

![Figure 2](image-url)

**Fig. 2.** Figure (a) shows the data from the numerical shear tests and the best linear fit. Figure (b) shows the linear approximation of the failure envelope from (a), the tensile strength of the material and the resulting Mohr-circle at the transition between tensile and shear failure.

<table>
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<th>analogue model</th>
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<td>Cohesion C</td>
<td>110 Pa</td>
<td>62 ± 5 Pa</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>41 Pa</td>
<td>33 ± 4 Pa</td>
</tr>
<tr>
<td>Bulk density $\phi$</td>
<td>860 kgm$^{-3}$</td>
<td>860 kgm$^{-3}$</td>
</tr>
<tr>
<td>Friction coefficient $\mu$</td>
<td>0.54</td>
<td>0.71</td>
</tr>
</tbody>
</table>
Fig. 3. Typical deformation patterns observed in the numerical experiments. Sharp color gradients in Figure (a) indicate localized deformation. Figure (a) shows the particles colored by their vertical displacement, Figure (b) shows the locations of bonds between particles breaking. The colors represent the time (in simulation time steps) at which the respective bond was broken.

Fig. 4. Main fault structures in the early stage of an analogue model. The underlying image is an enlarged section of Fig. 7C in Holland et al. (2006). The main faults are marked “A”, “B” and “C” analogous to the equivalent structures in the numerical model in Fig. 3(b).

record the breaking of the brittle-elastic inter-particle bonds. Tensile and shear failure modes were distinguished from the observation of particle velocities at the time of fracturing. The first fracture event observed is the formation of a sub-vertical tensile fracture starting at the surface and propagating downwards. This fracture is located up-dip from the projection of the trace of the basement fault to the top surface of the model. This fracture is marked “A” in Fig. 3(b). In most simulations there a second sub-vertical fracture (marked “B” in Fig. 3(b)) forms a little later and slightly further towards or in some cases down-dip surface projection of the basement fault. The second main feature is a curved fault initiating near the top of the basement fault and propagating upwards from there. The lower part of this fault is oriented sub-parallel to the basement fault whereas the middle section the fault steepens to become vertical and the upper part further curves away from the orientation at depth so that it dips in the opposite direction as the basement fault. This change in dip direction also results in a change in the style of movement from normal faulting at depth to reverse faulting near the surface of the model. Contrary to the tensile fractures forming at the surface, the primary fracture mechanism at this fault is shear failure. The point where this fault reaches the surface is marked “C” in Fig. 3(b). An additional feature which the numerical simulations share with both the analogue models (Holland et al., 2006; van Gent et al., 2010) and with field examples (Holland et al., 2006) is the existence of rotated triangular blocks next to the open tensile fractures.

To compare the locations of main fault structures, i.e. those marked “A”, “B” and “C” in Fig. 3(b), between the numerical and analogue model we are using data obtained from Holland et al. (2006). We have taken a section of Fig. 7C in that paper and identified the equivalent main fault structures “A”, “B” and “C” in the analogue model (Fig. 4). Measuring the horizontal locations of the faults relative to the basement fault we find that fault “A” is located 85 mm up-dip (i.e. left in Fig. 4) from the trace of the basement fault, fault “B” is located 43 mm up-dip and fault “C” 15 mm down-dip. The equivalent data have been determined for the numerical model by calculating the average fault locations from 3 model runs using the model with a basement fault dip of 60° in Section 4.2.3 (Fig. 5). We obtain a location 50 mm up-dip of the basement fault trace for fault “A”, fault “B” at 3 mm up-dip and fault “C” located 60 mm down-dip from the basement fault trace in the numerical model. This means that while the fault locations are offset between the numerical and the analogue model, the relative distances between the faults are similar.

4.2. Parameter space study

Of the many parameters which govern the behavior of the numerical model of the sandbox experiments we have chosen three to investigate their influence on the evolution of the fault structures in the model. First we perform a set of identical model simulations using different random realizations of the initial particle setup in order to obtain a qualitative estimate of the amount of variability induced by small heterogeneities in the material properties. After this we investigate how systematic variations in the material strength (tensile strength and cohesion) and the dip angle of the basement fault influence the evolving fault structures. There we also use multiple realizations of each model setup in order to constrain the variability.

4.2.1. Random realizations of granular packing

The material properties both of natural rock formations and of the analogue materials used in the laboratory experiments are generally not homogeneous. Due to the randomized setup procedure for the particle packing (Place et al., 2001) the numerical models also show heterogeneity in the material parameters at scales approaching the size of the DEM particles.

In order to test the sensitivity of model evolution to the small local disturbances caused by these heterogeneities and to evaluate the influence of the random initial particle packing on the fault structures generated in the model we have run a suite of several models with
identical macroscopic parameters and different initial particle arrangements (models 002–007 in Table 3). The results (Fig. 6) show that some features are robust such as the large scale fault patterns and the locations of earliest surface fault. Some features are less robust such as the existence of a 2nd sub-vertical surface fault and the shape and angle of main fault. In general it appears that in our models features which appear early in the faulting process are relatively robust whereas later features are more strongly influenced by small variations in the initial particle arrangement. A possible explanation for this observation would be that the differences in the early fault structures do influence the stress field in the model and that these changes provide additional source of variability for the later features.

4.2.2. Variation of cohesion

The bulk cohesion of the hemihydrate powder used in the laboratory experiments of Holland et al. (2006) and van Gent et al. (2010) is well known but the large scale bulk tensile strength in geologic structures is not so well known. Therefore we performed a series of simulations to test the effects of a variation of the cohesion relative to the experimental data. For the series of experiments shown in Fig. 7 the cohesion has been set to 0.1, 0.2, 0.5, 1.0, 2.0 and 5.0 times the experimental value, i.e. 11 Pa, 22 Pa, 55 Pa, 110 Pa, 220 Pa and 550 Pa respectively (models 008–013 in Table 4). The tensile strength scales accordingly, i.e. between 4.1 Pa for the material with a cohesion of 11 Pa and 205 Pa for the material with a cohesion of 550 Pa. The variation of the material strength has been achieved by scaling the failure threshold of the inter-particle bonds. The geometrical setup of these models is identical, using a dip angle of the basement fault of 60°. All models use the same initial particle arrangement in order to prevent variations in particle packing from influencing the fault structures developing.

The results show that the overall character of faulting changes from a shear zone at low cohesion to open (tensile) fractures in the upper part at medium to high cohesion (Fig. 7). The main right-trending fracture present in Fig. 3 does not appear at low cohesion (images a–c in Fig. 7), and changes its mechanism from primarily shear failure at medium cohesion to an open, tensile fracture at very high cohesion (Image f in Fig. 7).

For a more quantitative study of the influence of cohesion and tensile strength of the material the dependence of the maximum depth of the open fractures on the material strength has been investigated. The maximum depth at which fractures can remain open is determined by the stress conditions at which the transition between tensile and pure shear failure occurs. This transition condition is reached if the Mohr–circle touches the failure envelope in the tensile field but also in the shear field (Ferril and Morris, 2003; van Gent et al., 2010). If we assume a simple, linear Mohr–Coulomb failure criterion, such as the one obtained for our model material from a linear best fit to the data measured in the shear field and the tensile strength obtained in a direct tension test (Fig. 2(b)) we can estimate the vertical stress $\sigma_v$ at which this transition occurs from the equation

$$\sigma_v = \frac{-2C/tan\phi - T(1 + 1/sin\beta)}{1 - 1/sin\beta}$$  \hspace{1cm} (1)

where $C$ is the cohesion of the material, $T$ is the tensile strength and $\phi$ is the angle of internal friction. Assuming a constant mass density of the material in our model we can then calculate a theoretical estimate of the maximum depth $d_{max}$ of the open fractures from

$$d_{max} = \frac{\sigma_v}{g\phi}$$  \hspace{1cm} (2)

where $g$ is the gravitational acceleration and $\phi$ is the mass density of the material. Using the values obtained in Section 3.2, i.e. a tensile strength $T = -41$ Pa, a cohesion $C = 110$ Pa and an angle of internal friction $\phi = 28.5^\circ$, we obtain a vertical stress at the transition between shear and tensile failure $\sigma_v = 255$ Pa and therefore a transition depth $d_{max} \approx 32$ mm. From Eqs. (1) and (2) it can be seen that if the tensile strength and the cohesion are scaled by a common factor the transition depth will be scaled by the same factor. We can therefore expect a linear dependence of the depth of open fractures on the material strength in the models used in this section.

We did run three series of simulations, including the one shown in Fig. 7, where we used identical model geometry and varying material strength within each series. Between the series the particle packing was varied. The measured maximum depth to which the fractures stay open in each of the simulations shows the expected trend, i.e. the open fracture depth increases with increasing tensile strength and cohesion (Fig. 8). However, it does not exactly follow the linear relation predicted by Eqs. (1) and (2). For strength values up to twice the “baseline” values obtained in Section 3.2, i.e. $T \leq 80$ Pa, $C \leq 220$ Pa and therefore a depth of the open fractures of $d_{max} \approx 60$ mm, the match is quite good, taking the variability between the different random realizations of the model into account. For larger material strengths the observed depth of the open fractures begins to deviate from the theoretically predicted values. Tests using a larger model where the height of the sandbox was 250 mm instead of 150 mm in the other models suggests that this deviation might be a finite size effect. The depth of open fractures in this model (“Model III” in Fig. 8) stays very close to what would be theoretically predicted from Equations values 1 and 2 for greater material strength than what is observed for the models with a height of 150 mm.

4.2.3. Variation of basement fault angle

In order to evaluate the influence of the dip angle of the basement fault on the structure of the evolving fault zone we performed a suite of simulations (Fig. 9) using a model varying basement fault angles

![Fig. 5. Locations of the main faults depending on the dip angle of the basement fault. The positions are given relative to the surface projection of the basement fault with positive values denoting a position located down-dip from the trace of the basement fault. Error bars show minimum and maximum locations.](image-url)
between 40 and 90° (model parameters in Table 5). Those models used an identical initial particle arrangement and mechanical parameters. The variation of the fault angle does result in a systematic variation of the angle and location of main fault. There is also a systematic, albeit much smaller, variation of the location of the initial tensile surface fractures.

For a more quantitative study of the influence of the dip angle of the basement fault on the major structural features developing in the model we have plotted the location of the 3 main structures mentioned in Section 4.1, i.e. the tensile surface fractures (“A” and “B” in Fig. 3(b)) and the location where the main fault reaches the surface (“C” in Fig. 3(b)) depending on the basement fault angle (Fig. 5). Again, in order to obtain an estimate of the variability of the fault locations for models using different particle arrangements we have used data generated from 3 different models, using the same macroscopic model geometry but different random realizations of the initial particle packing.

Fig. 5 suggests that the location of the sub-vertical tensile faults “A” and “B” shows a small but systematic dependence on the dip angle of the basement fault. Fault “A” is moving away from the trace of the basement fault with increasing basement fault angle and always stays in a position clearly up-dip. Fault “B” is moving much less than fault “A”. Furthermore it is moving in the opposite direction, changing its location from nearly straight above the basement fault trace to a position slightly down-dip for high basement fault angles. Fault “C” moves by a much larger amount than the other faults but also shows a larger variability.

5. Discussion

The simulations of complex fault structures developing in cohesive materials have resulted in fault structures which are quite similar to those observed in natural prototypes and in scaled laboratory experiments despite the differences in the details of the material parameters used. In the analogue models the strength, i.e. cohesion and tensile strength, of the material increases with increasing depth and therefore burial stress. In the numerical models the material properties (i.e. cohesion and tensile strength) don’t significantly
change with depth. Therefore the transition between the failure modes from tensile to shear failure with increasing depth in the model is entirely due to the change in local stress conditions in the numerical model while it is also influenced by the depth dependent material properties in the analogue models. However, the increase in material strength with depth is much smaller than the depth-related increase of the mean stress (van Gent et al., 2010). Therefore the depth-dependent material properties will influence details like the depth of the transition, the results of the simulations shown here suggest that it doesn’t significantly change the overall character of the developing structures. In particular one would expect that in a model which includes a depth-dependent tensile strength increase the tensile to shear transition of the failure mode to occur at a deeper level.

One difference we observe between our numerical models and the analogue models of Holland et al. (2006) is that the main fault structures, while having a similar shape, appear in an offset location. In the numerical models the main faults are shifted up-dip relative to the basement fault compared with their location in the analogue experiments. It is not quite clear what causes this difference but it would be consistent with the fact that the early deformation features which appear before the formation of the main curved fault plane and might influence the location of the faults (see Fig. 6 in Holland et al., 2011) would be expected to have a shallower dip in the numerical models due to the lower friction angle compared to the analogue model. An additional aspect which is making the quantitative comparison between the analogue and the numerical models slightly more complicated is that we do not know much about the elastic parameters of the analogue material. Holland et al. (2006) state a bulk shear modulus of 50–80 kPa but neither Young’s modulus nor the Poisson ratio of the hemihydrate powder is well known.

The observation that the maximum depth of the open fractures is very well predicted by a linear dependence the cohesion (Fig. 8) as long as the model boundaries are far enough away from the fault zone suggests that the numerical models do have a predictive capability regarding the structure of natural fault zones as long as the material properties and the boundary conditions are sufficiently well known. We observe that the sub-vertical faults initiate at the model surface and propagate downwards, consistent with the
scale dependence of the heterogeneity of the material parameters in the initial conditions. A potential reason for this behavior is the solution of local deformation details diverges even for small differences in the minimum and maximum particle radii, realizations of the same model setup. If multiple model numbers are mentioned in a single table row then those models are different random realizations of the same model setup. With respect to the cohesion and tensile strength, both in Pa. If multiple model numbers are mentioned in a single table row then those models are different random realizations of the same model setup.

**Table 4**

Geometric and material properties of all simulation models used in Section 4.2.2 where H in the model height in mm, L is the model length in mm, $r_{\text{min}}$ and $r_{\text{max}}$ are the minimum and maximum particle radii, $\Phi$ is the dip of the basement fault in degrees and C and T are the cohesion and tensile strength, both in Pa. If multiple model numbers are mentioned in a single table row then those models are different random realizations of the same model setup.

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<th>Nr.</th>
<th>H [mm]</th>
<th>L [mm]</th>
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Discrete Element Models. Work by Koyama and Jing (2006) and Fakhimi and Gharahbagh (2010) has shown that the variability of the elastic and fracture properties of DEM model materials is dependent on the scale at which these parameters are considered. Koyama and Jing (2006) suggest that the “Representative Equivalent Volume” (REV), i.e. the minimum sampling volume beyond which the material properties remain constant, has a size of about 5 cm $\times$ 5 cm at a particle radius of 0.35–1 mm. Using the data given by Koyama and Jing (2006) for their particle packing this means that the suggested REV contains about 1500–3500 particles. While it might not be possible to apply this result directly to the particle packings used in this work, which use a wider particle size range, it does suggest that the overall material properties of our models can be considered to be largely independent of the concrete realization of the particle packing. However, the scale of the evolving fault structures in our model is similar to or smaller than the dimension of the REV suggested by Koyama and Jing (2006), resulting in a significant variation of the material properties at that scale. For higher resolution models the size ratio between the REV and the scale of the structures would be changed such that less variation of the material properties at the scale relevant for the structural evolution would be expected. However, the results of Koyama and Jing (2006) also suggest that it is not clear if the variation of the fracture parameters actually converges to zero with increasing sample volume (see Figs. 9 and 10 in Koyama and Jing, 2006). Fakhimi and Gharahbagh (2010) state that it does not, although for a slightly different model. This suggests that an exact geometrical match between a laboratory of field example and a simulation may not be possible, in particular because we have very little information about the small scale heterogeneity of the material parameters in the analogue materials. However, the modeling of more integral properties of the fault systems such as connectivity or permeability should be possible.

A major simplification of the models in this work compared to analogue is the use of 2D models. To evaluate the potential impact of the third dimension on the evolution of the faults we are considering the fault structures observed in the analogue models by van Gent et al. (2010), Holland et al. (2006) and Holland et al., (2011). In those models we see that while the main fault structures are not completely straight but slightly undulating they are largely sub-parallel to the basement fault, so the 2D models are a reasonable first order approximation. However, if we are looking at the analogue models in more detail, in particular with regard to smaller scale structures we see that the analogue models contain a wide range of real 3D structures, such as relay ramps which cannot be adequately represented in a 2D model or even a series of 2D models arranged as slices though a 3D volume.

### 6. Conclusions

The results obtained from a large number of numerical simulations have shown that the modeling results can be a good match of the lab results and field observations. The parameter space exploration performed using these simulations show that the main structural
elements of the evolving fault systems are robust even using only a rough approximation of the material properties and a relatively low resolution. The results obtained from this work show that there are a number of avenues for further exploration of the problem of normal faulting in cohesive materials using DEM simulations. Further work will need to be done on the inclusion of more detailed material properties, for example a closer match to the cam-clay-like failure envelopes of the gypsum-box experiments. In the future, these models will also be extended to 3D. A 3D model will be of particular interest because due to recently published work by Holland et al. (2011) using CT-scanning of analogue models there now are 3D data to compare the numerical modeling results with.

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References


