4. RESULTS AND DISCUSSION

4.1. CHARACTERIZATION OF ROUGHNESS, APERTURE AND TRANSMISSIVITY FIELDS USING SEMI-VARIOGRAMS

As for the characterization of roughness, the approach of the semi-variograms of the aperture and transmissivity fields was used. Figure 4.1 depicts the aperture and transmissivity distributions at four translational shear displacements. The arrow that appears below the distributions shows the direction of shear. In this Figure, it can be clearly seen that flow channels are generated perpendicular to the shear direction during shearing. On the other hand, Figure 4.2 shows the aperture and transmissivity distributions at four different rotary shear angles. The circular arrow that is placed below the low left-hand side corner of the distributions shows the direction of the rotary shear. All the semi-variograms in this chapter were produced by Koyama (2005) and are used here to highlight the effects of shear on flow and particle transport behaviours.

4.1.1. APERTURE

4.1.1.1. TRANSLATIONAL SHEAR

To begin with, Figure 4.3 shows the semi-variograms in the \(x\)-direction at different shear displacements. It can be seen that except for the first step of the shearing process, from 0.0 mm to 1.0 mm, the value of \(\gamma(l)\) increases with increasing shear displacement. This means that the aperture values become less correlated as the shear displacement increases. Furthermore, for translational shear displacements equal or greater than 2.0 mm, as it can be seen in Figure 4.5 (a), the semi-variogram adopts a shape with a maximum around 5 cm and a minimum around 9 cm, and the \(\gamma(l)\) increase greatly. The explanation to this shape lies on the channelling effect, which, as it can be seen in Figure 4.1 at 20.0 mm shear displacement, forms two channels with their respective contact areas. Therefore, the fracture is divided into four differentiated areas in the \(x\)-direction, two of large aperture values and two of small aperture values. Then, for a lag distance equal to one fourth of the fracture side, the aperture values are not correlated, because the contact areas and the channels are alternatively located. But, for a lag distance equal to half of the fracture, the aperture values are more correlated, because the contact areas and the channels coincide with each other. Finally, for larger lag distances, the correlation becomes smaller again because, while in the left-hand side boundary one can find large aperture values, in the right-hand side boundary a contact area can be found.

In view of the irregular shape of the semi-variograms, it has been decided not to fit them with a theoretical curve in order to define the range and the sill, because it would have resulted in an extremely subjective fitting. Furthermore, the size of the fracture is very reduced, smaller than 20 cm, so it cannot be ensured that for a larger sample the semi-variogram would reach a sill. It has to be noted that the \(\gamma(l)\) values change significantly during the shearing process, which means that the correlation length changes during the shearing process.
Figure 4.1. (a) Aperture and (b) transmissivity distributions of the numerical fracture sample at different translational shear displacements.
Figure 4.2. (a) Aperture and (b) transmissivity distributions of the numerical fracture sample at different rotary shear angles.
Results and Discussion

As for the $y$-direction, Figure 4.4 represents the semi-variograms of the aperture value at different shear displacements in the $y$-direction. Similarly to the $x$-direction, the $\gamma(l)$ value increases with increasing shear displacement, except at the start of the shear process, from 0.0 mm to 1.0 mm shear displacement. This means that the aperture values are less correlated with increasing shear displacement. Nevertheless, it has to be noted that the $\gamma(l)$ values have a narrow range, not being greater than 2.5 mm$^2$, which means that the aperture values have a high correlation for all lag distances. This fact can be also explained by the channelling effect that occurs during translational shear. As the channels and contact areas are created in the $y$-direction, the aperture values in the $y$-direction are very similar all along this direction, independently of the lag distance. From the observation of Figure 4.4, it can be seen that the $\gamma(l)$ values increase until they reach an almost constant value around 7 cm, especially for shear displacements larger than 5.0 mm, and then the semi-variograms present some oscillations that become more pronounced as shear displacement continues. Those oscillations might be due to the fact that the contact areas and channels do not follow a straight line and present some irregularities, causing a slight change in the correlation between aperture values for different lag distances.

Figure 4.3. Semi-variograms of the aperture value at different translational shear displacements in the $x$-direction.
Results and Discussion

Figure 4.4. Semi-variograms of the aperture value at different translational shear displacements in the \( y \)-direction.

Similar to the \( x \)-direction semi-variograms, the semi-variograms in the \( y \)-direction present shapes that are not very regular, especially for shear displacements larger than 5.0 mm. Although they seem to reach a constant value for lag distances larger than 7 cm, for larger lag distances there are some oscillations of the \( \gamma(l) \) values, and therefore, the fitting of a theoretical curve that would allow to define a range and a sill becomes quite subjective. Nevertheless, these oscillations may be due to the fact that for large lag distances, the measuring points is greatly reduced, having a minimum of 80 measures for a distance equal to the fracture size, i.e. 194 mm. Therefore, the accuracy of the results decreases. As in the \( x \)-direction, with a sample smaller than 20 cm, it can be said little things about what would be the tendency of the semi-variogram for bigger samples. Notwithstanding, if the lag distances larger than half of the fracture length are ignored, it could be said that a sill is reached for almost all cases, and that this sill becomes greater with increasing shear displacement. At the start of the shear process the sill would be small, around 3 or 4 cm, as it can be seen in more detail in Figure 4.5(a); for 10.0 mm shear displacement it would be around 5 cm; and for 20.0 mm shear displacement the sill would be found around 7 cm, which indicates that the correlation length increases during the shearing process in the \( y \)-direction.

With regard to the comparison of the \( x \) and \( y \)-direction, Figure 4.5 illustrates the semi-variograms of both \( x \) and \( y \)-direction at different shear displacements. As far as the initial stage of the translational process is concerned, it can be observed in Figure 4.5 (a) that there is a big change between 0.0 mm and 1.0 mm shear displacement in the \( x \)-direction, increasing significantly the aperture correlation for lag distances larger than 15 cm. On the other hand, in the \( y \)-direction the correlation is very similar between 0.0 mm and 1.0 mm shear displacement. But more important is the difference in the \( \gamma(l) \) values between the \( x \)-direction and the \( y \)-direction. This marked difference means that the aperture distribution changes significantly between these directions. After this initial shear displacement, the aperture values become less
correlated in both directions, but specially in $x$-direction, where the $\gamma(l)$ values increase rapidly. Figures 4.5 (b) and (c) show the shape of the semi-variograms in the $x$-direction that has been mentioned before, with a maximum around 5 cm and a minimum around 9 cm, which is a result of the channelling effect perpendicular to shear direction induced by translational shear. In contrast, the semi-variograms in the $y$-direction show a more regular shape and have much smaller $\gamma(l)$ values than in the $x$-direction, due to the fact that the channels are formed in the $y$-direction and then the aperture values are more correlated in this direction. Consequently, there is an induced anisotropy by translational shear.

(a)
Figure 4.5. Semi-variograms of the aperture values in the $x$-direction and $y$-direction at different translational shear displacements (a) from 0.0 mm to 2.0 mm, (b) from 3.0 mm to 7.0 mm and (c) from 10.0 mm to 20.0 mm.
4.1.1.2. ROTARY SHEAR

As far as the aperture values in the x-direction for rotary shear are concerned, Figure 4.6 shows the semi-variograms of the aperture values at different rotary shear angles. It can be seen that except for the first step of the rotary shear, the \( \gamma(l) \) values increase slightly with increasing rotary angles. Furthermore, for 10.0 degree rotary angle, the semi-variogram presents some oscillations that may be caused by the two contact areas that are formed during the rotary shear, one at the centre of the lower half of the fracture, and the other at the top left-hand side corner of the fracture. In comparison to the translational shear, it can be seen that the values of \( \gamma(l) \) are much smaller for rotary shear than for translational shear, which means that the aperture values are much correlated in the x-direction in the rotary shear than in the translational shear.

![Figure 4.6. Semi-variograms of the aperture values in the x-direction at different rotary shear angles.](image)

As it has been argued in the previous section, the semi-variograms have not been fitted by theoretical curves because of the irregularity of their shapes, it would have been a subjective task, implying a high degree of uncertainty. Therefore, one cannot define sills for these semi-variograms. Furthermore, for rotary shear the fracture size is even smaller than for translational case, making it more far-fetched to predict what would be the aperture correlation for larger lag distances. Apart from this, the fact that the aperture values are less correlated and present more irregular shapes with increasing rotary angles may imply a change in the correlation length during the shear process. Nevertheless, a sill could be approximated around 4 cm in all cases except for 10 degrees.

As for the aperture values in the y-direction, Figure 4.7 depicts some semi-variograms of the aperture values in the y-direction at different rotary shear angles. From this Figure, it can be seen that as in the x-direction, the aperture values become less correlated with increasing rotary angles. It can also be seen that almost all the curves present a decreasing...
tendency as they approach a lag distance equal to the sample size. This may be explained by the fact that the contact areas that are formed during the rotary shear are located close to the upper and lower boundaries, but not on them, so the aperture values become more similar in the boundaries than for a lag distance slightly smaller than the fracture size. For small rotary angles the semi-variograms have a quite regular shape, but as the rotary angle increases, its shape becomes more irregular and with constant oscillations. Nevertheless, the γ(l) values are smaller than 2 mm², indicating that the aperture values are quite correlated during the rotary shear process, compared to the γ(l) values during translational shear. In this case, due to the same reasons as in the other cases, the semi-variograms have not been fitted by any theoretical curve neither.

![Figure 4.7. Semi-variograms of the aperture values in the y-direction at different rotary shear angles.](image)

For the comparison between the x-direction and y-directions, Figure 4.8 shows the semi-variograms of both directions. For the small rotary angles, Figure 4.8 (a) shows that the semi-variograms in both directions have very similar values. Unlike translational shear, this means that both x-direction and y-direction have a similar aperture distribution during rotary shear. Therefore, rotary shear does not induce anisotropy in the aperture distribution. Nevertheless, the γ(l) values slightly increase with increasing rotary angles, showing that rotary shear produces a small reduction in correlation in the aperture values, which becomes more significant for large rotary angles. Looking the semi-variograms in detail, it can be seen that for lag distances shorter than around 7.5 cm, which is half of the fracture side, the x-direction is less correlated, but this situation shifts for lag distances between 7.5 cm and 12.5 cm, where x-direction is more correlated than y-direction. For lag distances larger than 11.5 cm the correlation in the y-direction increases, because the aperture values in the boundaries are more similar than for slightly shorter lag distance, due to the contact areas that are placed close to the upper and the lower boundaries. Nevertheless, these changes are very small, and it can be considered that both directions have a very similar aperture distribution.
However, for larger rotary angles, as it can be seen in Figure 4.8 (b), the semi-
variograms become more different between $x$-direction and $y$-direction for rotary angles larger
than 7.0 degree. While in the $y$-direction the $\gamma(l)$ values continue its tendency to increase, in
the $x$-direction the $\gamma(l)$ values have oscillations, and for lag distance larger than 5 cm, the
semi-variograms have a tendency to decrease in $\gamma(l)$, increasing the correlation between the
aperture values in the $x$-direction. Furthermore, it can also be seen that for small lag distances,
shorter than 4 cm, the aperture values in the $x$-direction become less correlated more rapidly
than in the $y$-direction. This behaviour for rotary angles equal or larger than 7.0 degree can be
explained by the location of the contact areas, because the contact area located in the centre of
the lower half of the fracture coincides in part with the contact area located in the upper half,
but there is not any connection between them in the $x$-direction.
Figure 4.8. Semi-variograms of the aperture values in the \( x \)-direction and \( y \)-direction at different rotary shear angles (a) from 0.0 degree to 3.0 degree and (b) from 5.0 degree to 10.0 degree.
4.1.2. TRANSMISSIVITY

4.1.2.1. TRANSLATIONAL SHEAR

As far as the transmissivity distribution is concerned, it is assumed to be related to the third power of the aperture, and therefore, a similar behaviour to the aperture distribution is expected. As for the \( x \)-direction, Figure 4.9 depicts the semi-variograms of the transmissivity at different translational shear displacements. It can be seen that the semi-variograms adopt similar shapes as those of aperture values in the \( x \)-direction. Nevertheless, the range of \( \gamma(l) \) values is much smaller, because the semi-variograms are calculated with the logarithm in base 10 of the transmissivity, which has a very wide range of values. Interestingly, the semi-variogram for 0.0 mm shear displacement presents \( \gamma(l) \) values greater than the majority of the semi-variograms for lag distance larger than 7 cm. This means that for zero shear displacement, the transmissivity values are less correlated than the transmissivity values during the shearing process for large lag distances. Furthermore, the semi-variograms between 2.0 mm and 10.0 mm shear displacements are very similar, indicating that the transmissivity has the same degree of correlation within this interval of shear displacements. This may be due to the fact that the channelling effect perpendicular to shear direction keeps the original shape during this shearing stage, with a similar distribution of the transmissivity values.

![Figure 4.9. Semi-variograms of the transmissivity values in the \( x \)-direction at different translational shear displacements.](image)

In this situation, it is also very subjective to try to fit these semi-variograms with theoretical curves that would give the ranges and the sills of the semi-variograms. However, some general trends can still be observed in Figure 4.9. Similar to the aperture semi-variograms, the effect that the channelling perpendicular to shear direction has on the transmissivity values is evident. Thus, there is less correlation between the transmissivity values for a lag distance of one fourth of the fracture side, a higher correlation for a lag distance of half of the fracture side, and again the correlation between the transmissivity...
values decreases for larger lag distances. This is due to the fact that two channels and two contact areas are formed equidistantly along the $y$-direction. Therefore, for a lag distance of one fourth of the fracture side, there will be on the one hand a high transmissivity value of a channel, and on the other hand a low transmissivity value of a contact area. In addition, for a lag distance equal to half of the fracture side, the high transmissivity values of the channels coincide between each other, as well as the low transmissivity values of the contact areas does. For lag distances larger than half of the fracture side, there will be again one high transmissivity value of a channel and on the other hand, a low transmissivity value of a contact area, and consequently, the transmissivity values will become less correlated.

As for the $y$-direction, the transmissivity semi-variograms have also a narrow range of $\gamma(l)$ values, as it can be seen in Figure 4.10. This narrow range of $\gamma(l)$ values is due to the fact that the channelling effect due to shearing is created in the $y$-direction, perpendicular to shear direction. Interestingly, the semi-variogram for zero shear displacement has a different shape, compared with other curves once translational shear has started. With increasing shearing displacements all the semi-variograms have a relatively similar shape and become less correlated as shear increases. This shows how significantly the fracture transmissivity changes due to shearing. Apart from this, it can be seen that lag distances close to the fracture side, i.e. 194 mm, have lower $\gamma(l)$ values than lag distances between one fourth and three fourths of the fracture side. This situation may be due to the fact that inside the contact areas there are some zones with quite different transmissivity values.

![Figure 4.10: Semi-variograms of the transmissivity values in the $y$-direction at different translational shear displacements.](image)

As for the comparison between the $x$-direction and the $y$-direction, Figure 4.11 shows the semi-variograms of both directions for different shear displacements. From Figure 4.11 (a), it can be seen that the semi-variograms in the $y$-direction have smaller $\gamma(l)$ values and similar shapes, while in the $x$-direction, though the semi-variograms are also similar among them, the $\gamma(l)$ values are larger, especially at zero shear displacement. For larger shear displacements,
Figure 4.11 (b) and 4.11 (c) show that the semi-variograms in the $x$-direction and the $y$-direction are similar in shapes and values within the same direction. Apart from this, when the lag distance is larger than 10 cm, the $x$-direction transmissivity values become less correlated than in the $y$-direction. This is due to the shear induced channelling that is formed perpendicular to shear direction, which produces a higher correlation between the transmissivity values for all lag distances in the direction perpendicular to shear. However, in the direction parallel to shear, $x$-direction, it produces a less correlated distribution of the transmissivity values.
Figure 4.11. Semi-variograms of the transmissivity values in the x-direction and y-direction at different translational shear displacements (a) from 0.0 mm to 2.0 mm, (b) from 3.0 mm to 7.0 mm and (c) from 10.0 mm to 20.0 mm.
4.1.2.2. ROTARY SHEAR

As far as the semi-variograms in the x-direction are concerned, once the rotary shear has started, the semi-variograms show similar shapes except for the 10.0 degree rotary angle, which changes its form and behaviour, as can be seen in Figure 4.12. The much higher $\gamma(l)$ values at zero rotary shear means that before shear takes place the transmissivity values are less correlated than those during shear. Furthermore, once shear starts, the $\gamma(l)$ values become much smaller and relatively constant for all lag distances. Therefore, the transmissivity values are highly correlated in the x-direction for all lag distances. As for the 10.0 degree rotary angle semi-variogram, it presents an oscillating behaviour that may be given by the formation of two contact areas, one in the top left-hand side corner, and the other at the centre of the lower half of the fracture. In general, once the rotary shear starts, the semi-variograms slightly increase their $\gamma(l)$ values with increasing rotary shear angles. As in the other cases, here it is not very appropriate to fit theoretical curves, because it would be very subjective and would introduce a degree of uncertainty in the range and sill values given by the theoretical curves. Nonetheless, sills may be determined around 4 cm for all curves except for 0 and 10 degrees, since these two cases are actually special. The zero degree represents the original uncorrelated nature, while the 10 degrees represents uncorrelation due to shearing. In general, rotary shear generates high correlation as proved by an almost isotropic and uniform flow field.

![Figure 4.12. Semi-variograms of the transmissivity values in the x-direction at different rotary shear angles.](image)

As for the y-direction, all the semi-variograms present similar shapes, with very small $\gamma(l)$ values, as it can be seen in Figure 4.13. In this situation, the semi-variogram for zero rotary angle has a quite similar shape and $\gamma(l)$ values compared with the other semi-variograms except for the case with 10 degree of rotary shear angle. All the semi-variograms show a tendency to slightly increase their $\gamma(l)$ values with increasing lag distances, but for lag distances close to the fracture side, i.e. 136 mm, the $\gamma(l)$ values drop rapidly. Moreover, the
\( \gamma(l) \) values between two consecutives rotary angles are also very close. This means that rotary shear maintains the transmissivity distribution in the \( y \)-direction when the rotary shear angle is not larger than 5 degrees. Furthermore, for lag distances larger than 11.5 cm, the \( \gamma(l) \) values decreases greatly in the semi-variograms in the \( y \)-direction. This may be due to the fact that the contact areas that are close to the upper and lower boundary respectively provoke that the correlation of the transmissivity values decreases for lag distances close to the fracture side, but for larger values, the effect of the contact areas disappears, because they are not next to the boundaries.

Comparing the semi-variogram behaviours between the \( x \)-direction and \( y \)-direction, all the semi-variograms for both directions present similar \( \gamma(l) \) values at every rotary shear displacement, as it can be seen in Figure 4.14. The semi-variograms in both directions have similar \( \gamma(l) \) values, which means that there is very little anisotropy when rotary shear occurs. In addition, it can be seen that the semi-variograms in the \( x \)-direction have slightly higher \( \gamma(l) \) values for lag distances up to 7 cm, which coincides with half of length of the fracture side, and then the semi-variograms in the two directions shift their relative locations with larger lag distances, and the transmissivity in the \( x \)-direction becomes more correlated than that in the \( y \)-direction. For larger rotary angles, as it can be seen in Figure 4.14 (b), the shape of the semi-variograms in both directions is essentially the same, but they become more separated as rotary shear increases. In general, it can be said that the \( \gamma(l) \) values are very small and although the semi-variograms in both \( x \)-direction and \( y \)-direction do not have similar shapes, they have very similar values, which shows that there is isotropic transmissivity field induced by rotary shear.
Figure 4.14. Semi-variograms of the transmissivity values in the $x$-direction and $y$-direction at different rotary shear angles (a) from 0.0 degree to 3.0 degree and (b) from 5.0 degree to 10.0 degree.
4.2. COUPLED FLUID FLOW AND PARTICLE TRANSPORT DURING SHEAR

In this section, the effects of shearing on fluid flow and particle transport are studied using numerical modelling. Different situations are considered, some of which cannot be reliably reproduced in laboratory tests, such as unidirectional flow perpendicular to the shear direction. Furthermore, this numerical approach allows us to reproduce and evaluate the paths followed by the particles, which is also a challenging problem to achieve at the laboratory.

4.2.1. UNIDIRECTIONAL FLOW PATTERNS

There are some studies for this kind of flow pattern, both experimental and numerical, but the combination of the processes of coupled stress-flow and particle transport have not been attempted. Some experimental studies considered coupled stress-flow test with normal and shear loading, but not transport (Yeo et al., 1998; Esaki et al., 1991, 1999; Lee et al., 2002), and others considered flow and transport processes, but not mechanical shear in experiments (Neretnieks et al., 1982; Abelin et al., 1991a, 1991b) and numerical modeling (Thompson, 1991; Cvetkovic et al., 1999; Wendland et al., 2002; Cheng et al., 2003). In this study, both aspects, i.e. coupled stress-flow and particle transport, are considered through numerical tests.

4.2.1.1. FLOW PARALLEL WITH SHEAR DIRECTION

This numerical test considers fluid flow and particle transport parallel with the translational shear direction, as outlined in Figure 4.15. This kind of flow pattern can be reproduced at laboratory with higher reliability, and several groups have studied the effects of shear on flow in rough fractures (Yeo et al., 1998; Esaki et al., 1999; Lee et al., 2002; Jiang et al., 2004), without considering particle transport. One exception is reported in Jiang et al. (2004), who used a transparent fracture replica to show tracer paths. In the current study, the numerical simulation is employed to study the evolution of the paths followed by the particles during shearing.

Figure 4.15. Outline of the coupled shear stress-flow test with unidirectional flow parallel with the shear direction.
Figure 4.16. Transmissivity distribution and particle paths of a numerical fracture sample at different shear displacements for flow parallel to shear direction.
Due to the roughness of the fracture surfaces, particles may change their paths during the shearing process. Figure 4.16 depicts the transmissivity and the particle paths at eight different translational shear displacements, ranging from 0.0 mm to 20 mm. In this numerical test, a hydraulic head of 1.0 m is applied in the right-hand side boundary of the sample fracture, while the left-hand side boundary has a hydraulic head of 0.0 m. The upper and lower boundaries of the fracture are no-flow boundaries. For the calculations, particles are placed in the right-hand side boundary, one particle in each element, resulting in a total of 80 particles.

From Figure 4.16, it can be seen that during the shearing process the contact areas are distributed but more oriented in the $y$-direction, i.e. perpendicular to the shear direction. This phenomenon creates channels, in the direction perpendicular to the shear, in which the permeability of the fracture is much higher than in the rest of the rough fracture. Thus, the particles, in order to avoid the contact areas, have to find the spaces between the contact areas, concentrating in the zones with higher transmissivity. This distribution may give a false impression of channelling, but it is due to the effect of flow and particles bypassing contact areas while keeping the general flow and particle transport paths in the $x$-direction.

The transmissivity of the rough fracture increases with increasing shear displacement, as it can be seen in Figure 4.16. The transmissivity is related to the velocity field, and the latter to the travel time of the particles. The higher the transmissivity is, the higher the velocity is, and the less time it takes to the particles to travel through the fracture. This effect can be studied with the aid of breakthrough curves. Figure 4.17 shows the breakthrough curves at different shear displacements. According to Bear (1988), a breakthrough curve shows the relationship between the relative tracer concentration and time, and allows to evaluate the dispersion of a tracer. In this study, the breakthrough curves show the relationship between the percentage of particles that reach the prescribed outflow boundaries and time.
Figure 4.17. Breakthrough curves for unidirectional flow parallel to shear direction (a) for small shear displacements and (b) for large shear displacements.

Figure 4.17(a) shows the breakthrough curves for small translational shear displacements. In general, it can be observed that the greater the shear displacement is, the less time it takes to the particles to travel through the fracture. For 0.0 mm shear displacement, i.e. before the shear process starts, the travel time is much longer. This means that shearing makes the rough fracture much more permeable. Note that it takes the same time to pass through the fracture for the faster 5% of the particles for 0.0 mm shear displacement than for the whole set of particles for 1.0 mm shear displacement. Furthermore, the slowest particle for 0.0 mm shear displacement spends four times the travel time of the slowest particle for 1.0 mm shear displacement. It can be seen from Figure 4.17 that the more shear displacement there is, the steeper the slope of the breakthrough curve is. This means that the time interval in which the vast majority of the particles arrive becomes smaller with increasing shear displacement. Usually, there are a few particles that travel faster than the bulk of particles, and a few ones that take more time to pass through the particle. For the former particles, this happens because some particles find fast paths without passing through any area with low permeability; and for the latter particles, the delay is due to the fact that they pass through some area with low transmissivity, taking more time to bypassing it.

With larger shear displacements, a similar trend can also be observed in Figure 4.17(b). The particles travel faster with increasing shear displacement, but the difference in time between them becomes smaller, especially for 15.0 mm and 20.0 mm shear displacement. In this case, there are a few particles that take much longer time to travel through the fracture. This can be explained by the formation of a contact area in the inflow boundary, i.e. the right-hand side boundary, which entraps these slow particles.
Table 4.1 shows some representative percentiles of the breakthrough curves represented in Figure 4.17. As far as the decrease in the travel time is concerned, for the percentile $t_{0.5}$, the ratio between $t_{0.5}$ at a given shear displacement and at the next step, is around 2.5 for shear displacements between 0.0 mm and 3.0 mm, but for greater shear displacements it becomes smaller, indicating that the most significant changes concerning travel time take place for smaller translational shear displacements. Furthermore, it can also be seen that the time intervals defined by the percentiles $t_{0.9}$ and $t_{0.1}$ decrease for increasing shearing displacement. For a statistical analysis, Table 4.2 and Figure 4.18 show the mean values and standard deviations of the travel time when fluid flow parallel to shear direction.

### Table 4.1. Percentiles of the travel time at different shear displacements for the case of flow parallel to shear displacement.

<table>
<thead>
<tr>
<th>Shear Displacement (mm)</th>
<th>t$_{0.01}$</th>
<th>t$_{0.1}$</th>
<th>t$_{0.5}$</th>
<th>t$_{0.9}$</th>
<th>t$_{1.0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0mm</td>
<td>106 s</td>
<td>315 s</td>
<td>388 s</td>
<td>605 s</td>
<td>1,190 s</td>
</tr>
<tr>
<td>1.0mm</td>
<td>50 s</td>
<td>119 s</td>
<td>150 s</td>
<td>220 s</td>
<td>294 s</td>
</tr>
<tr>
<td>2.0mm</td>
<td>21 s</td>
<td>50 s</td>
<td>60 s</td>
<td>76 s</td>
<td>91 s</td>
</tr>
<tr>
<td>3.0mm</td>
<td>6.9 s</td>
<td>19 s</td>
<td>23 s</td>
<td>30 s</td>
<td>42 s</td>
</tr>
<tr>
<td>5.0mm</td>
<td>0.5 s</td>
<td>6.7 s</td>
<td>8.5 s</td>
<td>10 s</td>
<td>28 s</td>
</tr>
<tr>
<td>10.0mm</td>
<td>0.2 s</td>
<td>2.0 s</td>
<td>2.8 s</td>
<td>3.5 s</td>
<td>4.6 s</td>
</tr>
<tr>
<td>15.0mm</td>
<td>0.2 s</td>
<td>1.1 s</td>
<td>1.8 s</td>
<td>2.5 s</td>
<td>5.1 s</td>
</tr>
<tr>
<td>20.0mm</td>
<td>0.7 s</td>
<td>0.8 s</td>
<td>1.3 s</td>
<td>2.0 s</td>
<td>20 s</td>
</tr>
</tbody>
</table>

### Table 4.2. Mean value and standard deviation of the travel time at different shear displacements for the case of flow parallel to shear displacement.

<table>
<thead>
<tr>
<th>Shear Displacement (mm)</th>
<th>Mean Value</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0mm</td>
<td>452 s</td>
<td>161 s</td>
</tr>
<tr>
<td>1.0mm</td>
<td>162 s</td>
<td>46 s</td>
</tr>
<tr>
<td>2.0mm</td>
<td>61 s</td>
<td>12 s</td>
</tr>
<tr>
<td>3.0mm</td>
<td>24 s</td>
<td>5.0 s</td>
</tr>
<tr>
<td>5.0mm</td>
<td>8.9 s</td>
<td>3.2 s</td>
</tr>
<tr>
<td>10.0mm</td>
<td>2.8 s</td>
<td>0.7 s</td>
</tr>
<tr>
<td>15.0mm</td>
<td>2.6 s</td>
<td>5.7 s</td>
</tr>
<tr>
<td>20.0mm</td>
<td>1.8 s</td>
<td>2.4 s</td>
</tr>
</tbody>
</table>

Figure 4.18. Mean values and standard deviations of the travel time during translational shear for flow parallel with shear displacement.
Figure 4.18 shows the effect that translational shear has on the travel time of the particles, decreasing drastically at the start of the shearing process. The mean travel time follows an exponential curve, with asymptote in 0 seconds for increasing shear displacements. As for the standard deviation of the travel time at different shear displacements, it has a similar tendency than the mean value, but decreases more drastically at the start of the shearing process and becomes almost constant for shear displacements larger than 3.0 mm, though with some oscillations at shear displacements larger than 15.0 mm, due to the significant delay of a small number of particles as mentioned before. This rapid decrease in the mean travel time is due to the increase in the transmissivity of the rough fracture during shear. As expected from the observation of the breakthrough curves, Figure 4.17, the standard deviation decreases with increasing shear displacements because the breakthrough curves become steeper as shear increases. Nevertheless, the long tails of some of the breakthrough curves for large shear displacements, such as 15.0 mm and 20.0 mm, imply a higher standard deviation, therefore breaking the decreasing tendency as shown in Fig. 4.18.

With regards to tortuosity, it is defined in this work as the quotient between the travel distance and the theoretical distance that the particle would travel if the surfaces of the fracture would have a constant separation between each other, which for unidirectional flow patterns coincide with the fracture side. The histograms of the tortuosity of the particle travel paths at different shear displacements are shown in Figure 4.19. At zero shear displacement (navy blue line in Figure 4.19(a)), the bulk of particles has a small mean tortuosity, as indicated by the highest mode, but there are some particles that follow quite tortuous paths. These tortuous paths starts to decrease when shear starts, as it can be seen for the 1.0 mm shear displacement case, in which there is only one mode and all particles travel through paths at most only 7% more than the theoretical travel distance of 194 mm, i.e. the length of the fracture, as a parallel plate model.Nevertheless, the larger the shear displacement becomes, the more the tortuosity increases. The histograms adopt bimodal shapes, such as 10.0 mm and 20.0 mm in Figure 4.19, giving an idea of how complex the particles’ paths become.

![Tortuosity histograms at different shear displacements for flow parallel to shear direction.](image-url)
The largest value for the tortuosity is around 1.2 for shear displacements equal and larger than 10.0 mm, which means that the particles travel a 20 % more distance than if they would go in a straight line following the flow direction. Figure 4.20 provides an idea of how much an increase of 20 % in the travel distance represents. If a particle would start in the low right-hand side corner of the fracture, and it was to follow a straight line, in the case that it would follow the diagonal of the square defined by the fracture, the tortuosity would be of 1.41, so it would have travel a 40 % more than if it would have just followed the low boundary of the fracture. Now, if the particle was reach a point of the left-hand side boundary situated at a height equal to two thirds the distance of the fracture side, it would have travelled a 20 % more than if it would have gone in a straight line following the flow direction.

Figure 4.20. Representation of equivalent tortuosity in a squared fracture sample.

This high tortuosity is caused by the complex paths that particles have to follow in order to bypass the contact areas that are formed perpendicular to shear direction, as it can be seen in Figure 4.16. With increasing translational shear displacement, it becomes more and more difficult to find a way to bypass the contact areas formed during the shear process, but the vast majority of the particles always find their ways in such tortuous path geometry. For the cases of 10.0 mm, 15.0 mm and 20.0 mm shear displacements in Figure 4.16, it can be seen how particles seek the least resistant paths and move towards the upper boundary while shearing close the contact areas that are found to the left of the centre of the fracture.
4.2.1.2. FLOW PERPENDICULAR TO SHEAR DIRECTION

This particular numerical test has a special interest because it is really difficult to reproduce reliable boundary conditions for this type of flow in laboratory. This is because it is necessary to seal the fractures in the direction parallel with the flow direction, which is almost impossible, especially when large shear displacement is required. Yeo et al. (1998) performed an experiment in which fluid flow perpendicular to shear direction was considered, for up to 2 mm of shear displacement. Some other studies (Jing et al., 2004; Koyama et al., 2005) stated that this shortcoming in the experimental test may lead to significant underestimation of the fracture transmissivity of a rough rock fracture during shearing processes, due to the fact that the effect of the shear dilation on flow in the direction perpendicular to shear is much greater than that in the direction parallel to shear direction. Figure 4.21 shows an outline of an imaged experimental conditions for this unidirectional flow pattern.

![Image of flow pattern](image)

Figure 4.21. Outline of the coupled shear stress-flow unidirectional flow perpendicular to the shear direction.

As it has already been mentioned in the previous section, during the translational shear, channels are formed in the direction perpendicular to shearing. Figure 4.22 shows the transmissivity and the paths followed by the particles at different shear displacement. As it also happens in the case of flow parallel with the shear direction, Figure 4.22 shows a great change in the particles’ paths between the 0.0 mm and the 1.0 mm shear displacement. When shear starts, the particle paths distribute more uniformly than before shear occurs. But, for larger shear displacement, the particle paths rearrange again, concentrating in the channels, which have a higher transmissivity than the rest of the rough fracture. From Figure 4.22, it seems that the channelling effect starts to be significant from 5.0 mm shear displacement onwards. Furthermore, for the 20.0 mm shear displacement case, two main channels can be clearly seen in the direction perpendicular to shear direction.
Figure 4.22. Transmissivity distribution and particle paths of a numerical fracture sample at different shear displacements for flow perpendicular to shear flow.
As for the breakthrough curves, which can be seen in Figure 4.23, they follow a similar trend as in the case of flow parallel with shear direction. However, some differences can still be detected. Firstly, unlike flow parallel with shear direction, there are always a few particles that travel in very short time, which means that there are at least a few particles that find fast ways for all the steps of the shear process. On the other hand, for small shear displacements, as it can be seen in Figures 4.17 (a) and 4.23 (a) and Tables 4.1 and 4.3, though once the shear has started the $t_{0.5}$ is smaller for the case of flow perpendicular to shear direction, there are still a few particles that take more time in crossing the fracture than in the case of flow parallel with shear direction. Thus, the range of travel time is wider for small shear displacements for the flow perpendicular to shear direction than that for the flow parallel to it. Similarly, as it can be seen in Table 4.3, the range of travel time values defined by the percentiles $t_{0.1}$ and $t_{0.9}$ is wider for the flow perpendicular to shear direction, but the values of $t_{0.9}$ are very similar when shear displacements are larger than 1.0 mm, with a tendency to decrease for the flow perpendicular to shear direction. This signifies that in the case of flow perpendicular to shear direction, a larger number of particles travel faster than in the case of flow parallel to shear direction. However, 90% of the particles will arrive at the outflow boundary at a similar time. This phenomenon may be explained as some particles, when they are released in the inflow boundary, i.e. the lowest boundary, are placed near one of the contact areas formed during shear, and some time is needed to find a least resistant path, while others travel very fast in the channels. Interestingly, in the case of flow perpendicular to shear direction with larger shear displacements, as it can be seen in Figure 4.23 (b), no particle is significantly delayed. This may be explained by the fact that there are no contact areas in the inflow boundary, and the particles that are placed at their starting points in low transmissivity areas can move quite rapidly from them.

(a)
Results and Discussion

Figure 4.23. Breakthrough curves for unidirectional flow perpendicular to shear direction (a) for small shear displacements and (b) for large shear displacements.

Overall, the breakthrough curves are displaced to the left and become steeper for increasing shear displacement. Almost any particle has significant delays, due to the existence of the channelling effect that occurs during shearing. Finally, it should be noted that at 0.0 mm shear displacement, the particles in the case of flow perpendicular to shear direction take more time in passing through the fracture compared to the case of flow parallel with the shear direction. It becomes, however, the other way around for large shear displacement, such as 15.0 mm or 20.0 mm, representing the significant effect of the translational shear on the particle transport in the case of flow perpendicular to shear.

Table 4.3. Percentiles of the travel time at different shear displacements for the case of flow perpendicular to shear displacement.

<table>
<thead>
<tr>
<th>t_0.01</th>
<th>0.0mm</th>
<th>1.0mm</th>
<th>2.0mm</th>
<th>3.0mm</th>
<th>5.0mm</th>
<th>10.0mm</th>
<th>15.0mm</th>
<th>20.0mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>t_0.1</td>
<td>42 s</td>
<td>30 s</td>
<td>8.4 s</td>
<td>3.3 s</td>
<td>1.1 s</td>
<td>0.3 s</td>
<td>0.1 s</td>
<td>0.1 s</td>
</tr>
<tr>
<td>t_0.5</td>
<td>427 s</td>
<td>109 s</td>
<td>47 s</td>
<td>17 s</td>
<td>5.4 s</td>
<td>1.6 s</td>
<td>0.9 s</td>
<td>0.6 s</td>
</tr>
<tr>
<td>t_0.9</td>
<td>770 s</td>
<td>316 s</td>
<td>74 s</td>
<td>35 s</td>
<td>9.4 s</td>
<td>3.0 s</td>
<td>1.9 s</td>
<td>1.3 s</td>
</tr>
<tr>
<td>t_1.0</td>
<td>1,770 s</td>
<td>477 s</td>
<td>284 s</td>
<td>190 s</td>
<td>64 s</td>
<td>6.4 s</td>
<td>3.2 s</td>
<td>3.5 s</td>
</tr>
</tbody>
</table>

Table 4.4. Mean value and standard deviation of the travel time at different shear displacements for the case of flow perpendicular to shear displacement.

<table>
<thead>
<tr>
<th>Mean value</th>
<th>0.0mm</th>
<th>1.0mm</th>
<th>2.0mm</th>
<th>3.0mm</th>
<th>5.0mm</th>
<th>10.0mm</th>
<th>15.0mm</th>
<th>20.0mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value</td>
<td>472 s</td>
<td>145 s</td>
<td>51 s</td>
<td>20 s</td>
<td>6.5 s</td>
<td>1.7 s</td>
<td>1.0 s</td>
<td>0.7 s</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>314 s</td>
<td>106 s</td>
<td>39 s</td>
<td>22 s</td>
<td>7.9 s</td>
<td>1.1 s</td>
<td>0.7 s</td>
<td>0.6 s</td>
</tr>
</tbody>
</table>
Results and Discussion

As shown in Fig. 4.24 and Table 4.4, respectively, the mean value of the travel time, as well as its standard deviation, decreases exponentially, with an asymptote in 0 seconds. In this case, there is not any particle entrapped in a contact area, so the standard deviation does not present any oscillation, having instead a slightly decreasing tendency for larger shear displacements. This is also reflected in the trend of the breakthrough curves becoming steeper with increasing shear displacements.

The comparison of Tables 4.2 and 4.4, and Figures 4.18 and 4.24 illustrates more clearly the effect of translational shear on particle transport. Before shear starts, i.e. 0.0 mm, the mean value of the particle travel time with flow parallel with shear direction is smaller than that with flow perpendicular to shear direction. With increasing shear displacements the mean value of the travel time is smaller for the case of flow perpendicular to shear displacement. This is due to the channelling effect in the direction perpendicular to shear displacement, which creates a high transmissivity channels through which particles can travel fast and without being delayed by bypassing low transmissivity areas, as it happens when the fluid flow is parallel with shear displacement. The standard deviation of the travel time, for shear displacements up to 10.0 mm, has larger values when flow is perpendicular to shear direction. But for shear displacements larger than 10.0 mm, the formation of larger contact areas and channels changes the situation. All in all, particles travel faster and with a smaller standard deviation when fluid flow is perpendicular to shear direction.

Figure 4.24. Mean value and standard deviation of the travel time during translational shear for flow perpendicular to shear displacement.
Figure 4.25. Comparison of travel time histograms between $x$- and $y$-directions at different shear displacements (a) 0.0 mm, (b) 1.0 mm, (c) 5.0 mm and (d) 20.0 mm shear displacement.
Results and Discussion

Figure 4.25 shows the comparison, between the $x$- and $y$-directions, of the histograms of the particles travel time at different translational shear displacement. It can be seen how the behaviour of particles in each direction changes during the shearing process. Before shear starts, Figure 4.25 (a), the two histograms show completely different shapes, but similar travel time for the peaks. The histogram in the $x$-direction has a sharp peak, indicating that a great number of particles arrive in a smaller time interval. On the other hand, in the $y$-direction (perpendicular to the shear direction), particles arrive mainly in two time intervals, as indicated by the double peak of the curve, one around 100 seconds, and the other around 500 seconds, respectively. It can also be seen that in the $y$-direction, the delayed particles take 50% more time than the slowest particle in the $x$-direction. Once shear starts, Figure 4.25 (b), the travel times are reduced significantly, and it can be observed that the particles in the $y$-direction travel faster than in the $x$-direction, due to the channelling created perpendicular to the shear direction. Nevertheless, the peak in the $x$-direction is sharper that in the $y$-direction, where two peaks are still kept, indicating that most of the particles still travel at a similar speed along the fracture. As for the delayed particles in the $y$-direction, there are still a few particles that take more time than the slowest particle in the $x$-direction. This may be due to the fact that 1.0 mm shear displacement is not enough to create large channels through which the particles can travel easily, and a few of them are entrapped in low transmissivity areas.

With a shear displacement of 5.0 mm, as it can be seen in Figure 4.25 (c), the particles in both directions have one-mode histograms, with a few delayed ones. It can be seen that in the $y$-direction the particles start arriving earlier than in the $x$-direction, but there are still a few more particles that take more time that the ones in the $x$-direction. The mode in the $x$-direction is sharper than that in the $y$-direction, indicating different channel velocities in the $y$-direction that leads to a wider range of travel time values. Finally, for 20.0 mm shear displacement, Figure 4.25 (d), it is clearer that the particles in the $y$-direction, travel much faster than the particles in the $x$-direction. The two peaks in the $y$-direction represent the arrival times of the particles through two main channels formed in this direction. At this shear displacement, there are more particles delayed in the $x$-direction, which takes twice the time of the slowest particles in the $x$-direction. In general, these figures show how the translational shear affects the behaviour of the particle movements in the $x$- and $y$-directions by creating high transmissivity channels in the $y$-direction through which the particles can travel faster.

Figure 4.26 shows the histograms of the tortuosity of the particle travel paths at different shear displacement when fluid flow is perpendicular to shear direction. It can be seen that the range of the tortuosity values is quite limited, from 1 to 1.1. This means that at most, a particle travels a distance 10% larger than the fracture length. This small increase in the travel paths with this flow pattern may be due to the existence of the channelling in the $y$-direction, which forms high transmissivity paths through which particles travel more smoothly. It can also be seen in Figure 4.26 that at the start of the shearing process, i.e. at 1 mm shear displacement, the majority of the particles have a very similar travel distance, being not longer than a 4% of the fracture length, indicating a quite homogeneous transport field due to shearing.

As shearing becomes larger, the histograms start to adopt a bimodal shape, as it can be seen in Figure 4.26 for 3.0 mm and 5.0 mm shear displacements. This may be explained by the formation of a high transmissivity channel in the neighbourhood of the left-hand side boundary of the fracture, in which the particles follow an almost straight path. At 5.0 mm shear displacement, tortuosity of paths of a few particles starts to increase slightly, which may be due to the channelling formation, indicating that some particles tried alternative paths until they find a high transmissivity channel. For shear displacements equal and larger than 10.0
mm, while the mode of small tortuosity values due to the particles placed near the left-hand side boundary remains, other particles increase their tortuosity up to an 8% longer than the fracture length. Those particles, as it can be seen in Figure 4.22, have to go around a contact area, and therefore, their tortuosity increase. Recalling Figure 4.20, it can be seen that an increase of an 8% in the travel distance in comparison to the fracture length implies that the particle would travel a distance close to the hypotenuse of the rectangle triangle with one side equal to the fracture side, and the other equal to half the fracture side.

Figure 4.26. Tortuosity histograms at different shear displacements for flow perpendicular to shear direction.

In comparison with the tortuosity of the particle travel paths in the case of flow parallel with the shear direction, it can be seen, from Figure 4.27, that the particle travel paths, when the flow is perpendicular to the shear direction, have smaller tortuosity. This is due to the fact that the particles can travel a shorter way through the created channels. In other words, when fluid flows parallel with the shear direction, the contact areas are distributed perpendicularly to the flow direction, so the particles bypass the low transmissivity zones, which implies longer travel paths. Interestingly, at the start of the shearing process, for both flow patterns the tortuosity becomes smaller than before the shearing, and the histograms have a unique narrow mode, Figure 4.27 (a) and 4.27 (b), though the values of the tortuosity are smaller when fluid flow is perpendicular to shear direction. Furthermore, for larger shear displacements, the histograms adopt more irregular shapes for both flow patterns, due to the increase in complexity of the transmissivity distribution that occurs during shear.
Results and Discussion

(a) and (b) show the frequency distribution of tortuosity for different thicknesses.

Frequency (%) vs. Tortuosity for (a) x_00mm and y_00mm and (b) x_1mm and y_1mm.
Figure 4.27. Comparison of tortuosity histograms at different shear displacement (a) 0.0 mm, (b) 1.0 mm, (c) 5.0 mm and (d) 20.0 mm shear displacement.
4.2.2. BI-DIRECTIONAL FLOW PATTERN

Bi-directional flow is an innovative approach that provides a more realistic test conditions. Koyama et al. (2004) used this flow pattern to study shear-induced anisotropy and heterogeneity of fluid flow in a single rough rock fracture with translational shear displacement. In the current study, particle transport is introduced to further this study. The boundary conditions that govern this flow pattern are difficult to perform at laboratory. Under such test conditions, a smooth parallel plate fracture will generate particle travel paths as presented in Figure 4.28.

Figure 4.28. Particle paths in a parallel plate fracture under bi-directional flow pattern.

However, for rough fractures undergoing shearing, the particle travel path distribution will vary significantly, as it can be seen in Figure 4.29. At 0.0 mm shear displacement, most of the particles reach the left-hand side boundary, with the predominating flow in the x-direction. This behaviour shifts very rapidly with shear. At a shear displacement of 2.0 mm there are more particles reaching the upper boundary rather than the left-hand side boundary. This may be a result of the dilatancy, which results in the channelling effect in the direction perpendicular to shear. From Figure 4.29, it is very clear to see how, for very small shear displacements, shear affects flow and particle transport. At 5.0 mm shear displacement, the formation of a channel in the y-direction is shown and it continues to grow with increasing shear displacements, such as at 10.0 mm, 15.0 mm and 20.0 mm. The numerical modelling of this test condition helps to highlight the significant shortcomings of the conventional shear-flow test in laboratory with one-directional flow.
Figure 4.29. Transmissivity distribution and particle paths of a numerical fracture sample at different shear displacements for bi-directional flow.
As far as the travel time is concerned, the directional tendencies that follow the particles has been studied by means of considering separately the particles that reach the left-hand side boundary and those that reach the upper boundary. Figure 4.30 shows the breakthrough curves of the particles that reach the left-hand side boundary (x=0 mm), those that reach the upper boundary (y = 194 mm) and the total amount of particles at different shear displacements. As shown in Figures 4.28 and 4.29, the particles travel with different paths of different lengths, so it is expected that some particles will have a really small travel time because of short travel distances.
Results and Discussion

(c) 

(d)
Results and Discussion

Figure 4.30. Breakthrough curves considering the amount of particles that reach each outflow boundary at different shear displacements (a) 0.0 mm, (b) 1.0 mm, (c) 3.0 mm, (d) 5.0 mm, (e) 10.0 mm and (f) 20.0 mm.
As shown in Figure 4.30 (a), at zero shear displacement, the predominant flow is in the x-direction, attracting more than two thirds of the total amount of particles. At 1.0 mm shear displacement, Figure 4.30 (b), the travel time becomes shorter, but there are a few particles that are delayed in the y-direction. As for the number of particles that reach each boundary, the percentage of particles that reach the left-hand side boundary is reduced to less than two thirds of the total amount of particles. At 2.0 mm shear displacement, there is a shift in the predominant transport direction.

From 1.0 mm to 3.0 mm shear displacements, Figures 4.30 (b) and 4.30 (c), the percentages of particles that reach each boundary change drastically. While around two thirds of the particles reach the left-hand side boundary at 1.0 mm shear displacement, it is the opposite situation at 3.0 mm shear displacement, i.e. two thirds of the particles reach the upper boundary. Furthermore, due to the increase in the transmissivity originated by the shear process, the travel time is reduced significantly, showing the great effect that shear has on transport. Nevertheless, no normal loading was considered in this study, which means that this results overestimate the travel time reduction. Apart from that, it can also be seen from Figures 4.30 (c), 4.30 (d), 4.30 (e) and 4.30 (f) that the vast majority of the particles that reach the left-hand side boundary travel faster than the first particles that arrive at the upper boundary. This is due to the higher transmissivity zone at the lower-left part of the fracture sample in comparison to the low transmissivity zones that are found near the upper right-hand side boundary. In addition, for shear displacements greater than 5.0 mm, as the particles that reach the left-hand side boundary spend a very short time travelling in comparison to bulk of particles that reach the upper boundary, the shape of the breakthrough curve of the total set of particles is almost identical to the breakthrough curve of the particles that reach the upper boundary.

Table 4.5 presents the percentiles of the breakthrough curves shown in Figure 4.30 for the total amount of particles as well as for the particles that reach the left-hand side and the upper boundaries. From Table 4.5, it can be seen that the percentage of particles that reach each boundary becomes very similar for shear displacements greater than 5.0 mm, though it has a tendency towards increasing the number of particles that reach the upper boundary, indicating how rapid translational shear provokes a greater flow and transport perpendicular to the shear direction than those parallel with the shear direction. For large shear displacements, as it can be seen in Figures 4.30 (e) and 4.30 (f) and in Table 4.5, most of the particles can find a fast path without being entrapped in any low transmissivity area, as indicated by generally short travel time. Nevertheless, at both 10.0 mm and 20.0 mm shear displacements, the time that takes to the slowest particle to arrive at the upper boundary is twice the time that takes for 90 % of the particles to reach an outflow boundary. This is due to the fact that some of particles have to travel a longer distance than the others may find some difficulties in bypassing some low transmissivity zones. Similarly, at 5.0 mm shear displacement, as it can be seen in Figure 4.30 (d), there is one particle that takes four times of the time that the 90 % of the particles take to reach an outflow boundary, because it is entrapped in a low transmissivity zone near the right-hand side boundary.
Table 4.5. Percentiles of the breakthrough curves at different shear displacement for bi-directional flow for (a) the total amount of particles, (b) the particles that reach the left-hand side boundary and (c) the particles that reach the upper boundary.

(a)

<table>
<thead>
<tr>
<th>total</th>
<th>0.0mm</th>
<th>1.0mm</th>
<th>3.0mm</th>
<th>5.0mm</th>
<th>10.0mm</th>
<th>20.0mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(t_{0.1})</td>
<td>1.0 s</td>
<td>0.5 s</td>
<td>0.1 s</td>
<td>0.1 s</td>
<td>0.0 s</td>
<td>0.0 s</td>
</tr>
<tr>
<td>(t_{0.5})</td>
<td>340 s</td>
<td>79 s</td>
<td>10 s</td>
<td>3.2 s</td>
<td>1.1 s</td>
<td>0.5 s</td>
</tr>
<tr>
<td>(t_{0.9})</td>
<td>605 s</td>
<td>260 s</td>
<td>49 s</td>
<td>16 s</td>
<td>3.0 s</td>
<td>1.2 s</td>
</tr>
<tr>
<td>(t_{1.0})</td>
<td>1,060 s</td>
<td>530 s</td>
<td>70 s</td>
<td>61 s</td>
<td>6.9 s</td>
<td>2.9 s</td>
</tr>
</tbody>
</table>

(b)

<table>
<thead>
<tr>
<th>(x=0\text{mm})</th>
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<th>1.0mm</th>
<th>3.0mm</th>
<th>5.0mm</th>
<th>10.0mm</th>
<th>20.0mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(t_{0.1})</td>
<td>1.8 s</td>
<td>0.5 s</td>
<td>0.0 s</td>
<td>0.0 s</td>
<td>0.0 s</td>
<td>0.0 s</td>
</tr>
<tr>
<td>(t_{0.5})</td>
<td>440 s</td>
<td>110 s</td>
<td>3.0 s</td>
<td>0.8 s</td>
<td>0.2 s</td>
<td>0.1 s</td>
</tr>
<tr>
<td>(t_{0.9})</td>
<td>650 s</td>
<td>275 s</td>
<td>17 s</td>
<td>3.2 s</td>
<td>0.8 s</td>
<td>0.2 s</td>
</tr>
<tr>
<td>(t_{1.0})</td>
<td>1,060 s</td>
<td>315 s</td>
<td>31 s</td>
<td>8.2 s</td>
<td>1.1 s</td>
<td>0.4 s</td>
</tr>
<tr>
<td>% of particles</td>
<td>73.75 %</td>
<td>63.75 %</td>
<td>33.75 %</td>
<td>28.75 %</td>
<td>26.25 %</td>
<td>23.75 %</td>
</tr>
</tbody>
</table>

(c)

<table>
<thead>
<tr>
<th>(y=194\text{mm})</th>
<th>0.0mm</th>
<th>1.0mm</th>
<th>3.0mm</th>
<th>5.0mm</th>
<th>10.0mm</th>
<th>20.0mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(t_{0.1})</td>
<td>0.2 s</td>
<td>0.3 s</td>
<td>0.7 s</td>
<td>0.7 s</td>
<td>0.3 s</td>
<td>0.3 s</td>
</tr>
<tr>
<td>(t_{0.5})</td>
<td>84 s</td>
<td>28 s</td>
<td>20 s</td>
<td>6.2 s</td>
<td>1.6 s</td>
<td>0.6 s</td>
</tr>
<tr>
<td>(t_{0.9})</td>
<td>450 s</td>
<td>180 s</td>
<td>55 s</td>
<td>18 s</td>
<td>4.0 s</td>
<td>1.8 s</td>
</tr>
<tr>
<td>(t_{1.0})</td>
<td>515 s</td>
<td>530 s</td>
<td>70 s</td>
<td>61 s</td>
<td>6.9 s</td>
<td>2.9 s</td>
</tr>
<tr>
<td>% of particles</td>
<td>26.25 %</td>
<td>36.25 %</td>
<td>66.25 %</td>
<td>71.25 %</td>
<td>73.75 %</td>
<td>76.25 %</td>
</tr>
</tbody>
</table>

4.2.3. RADIAL FLOW PATTERNS

Radial flow patterns are usually performed in bored circular core samples. However, coupled stress-flow test with circular cores considering shear, whether translational or rotary, are not very usual (Olsson, 1992; Olsson et al., 1993; Cheon et al., 2002). Although a circular sample would be more appropriate for numerical modelling as the one presented in this thesis with flow from centre, however, experimental data on roughness and aperture evaluation with circular samples are not available. Therefore, square samples as used before were used for simulating rotary shear while keeping the nominal contact area constant. The theoretical particle paths distribution considering a parallel plate fracture is represented in Figure 4.31. For the case of particle transport with radial flow, two shear patterns are considered, translational shear and rotary shear, and results will be compared between the two cases.
4.2.3.1. TRANSLATIONAL SHEAR

Though radial flow seems to be easier to implement in circular samples (Gentier et al., 1996), some studies have been done using rectangular specimens (Yeo et al., 1998; Esaki et al., 1999). In this study, a squared sample was used in order to study the effect of translational shear on radial flow. As it also happens in the unidirectional and bi-directional flow patterns during translational shear, channelling is expected to influence the behaviour of the particle paths.

Figure 4.32 shows the transmissivity distribution and the paths that particles follow at different translational shear displacements, from 0.0 mm to 20.0 mm. The initial distribution of the particle paths is almost isotropic, but with increasing shear displacement the distribution becomes more anisotropic, being quite different from the idealized case as shown in Figure 4.31. For large shear displacements, it can be seen how the particles travel through the channel formed in the y-direction, without too much lateral spreading, especially those starting in the lower boundary of the central hole. Nevertheless, due to the formation of a large contact area in the left side of the fracture sample, close to the hole, the particles placed more to the left of the upper boundary of the hole are deviated to the left side of the fracture. Similarly, the particles that start in the left-hand side boundary of the hole travel to the left through a zone with higher transmissivity placed between two of these contact areas in the left side of the fracture.
Figure 4.32. Transmissivity distribution and particle paths of a numerical fracture sample at different shear displacements for radial flow under translational shear.
As far as the breakthrough curves are concerned, they show the directional behaviour of the particles travel time during the shearing process (Fig. 4.33). Firstly, at zero shear displacement, the first particles that arrive at an outflow boundary are those that travel to the left, probably because that (cf. Fig. 4.32) there is an area of higher transmissivity in the left part of the fracture, and therefore, the particles travel faster through it. Furthermore, the number of particles that reach the left-hand side boundary is greater than the number of particles that start at the left-hand side inflow boundary, showing the capacity of attraction that this high transmissivity area has on its surrounding area. The particles that spend more time travelling are those travelling to the lower boundary of the fracture. Moreover, there are fewer particles that reach the boundaries in the $y$-direction, and the slowest particle in this direction is slower than the slowest particle in the $x$-direction. This indicates that at zero shear displacement, the transport in the $x$-direction predominates.

Once the translational shear starts, the travel times are reduced greatly. The particles begin to arrive at the different outflow boundaries at similar time, around 30 seconds, and 85% of the particles arrive in less than 100 seconds. There are a few particles that take quite much more time to reach an outflow boundary, especially for the left-hand side boundary, in which for 1.0 mm shear displacement, the slowest particle to reach this boundary takes more than twice the time that the slowest particle takes at zero shear displacement. This may be due to the fact that a contact area perpendicular to shear direction seems to be formed to the left of the centre of the fracture. Nevertheless, the left part of the fracture, to the left of the just mentioned contact area, still has a high transmissivity. As it happened at zero shear displacement, the left-hand side boundary receives more particles than the number of particles that start at the left-hand side inflow boundary.

With increasing shear displacements, the transmissivity increases in areas pointing to the $y$-direction, i.e. perpendicular to shear displacement. At 3.0 mm shear displacement, this effect results in the particles travelling towards the lower boundary presenting smallest travel time. Some particles that travel towards the upper boundary have slower velocity and a few of them are deviated towards the left hand side boundary, due to the contact area located close to the left of the centre (Fig. 4.32). This contact area also affects the particles that travel towards the left-hand side boundary, with a few of them being significantly delayed, more than twice the time it takes to the slowest particle in the $y$-direction. Apart from this, the particles placed in the upper part of the right-hand side inflow boundary reach the upper outflow boundary. This may be due to the fact that with increasing shear displacement, the flow in the $y$-direction has higher velocity compared to the flow in the $x$-direction.

At 5.0 mm shear displacement, the fastest particles continue to be those that travel towards the lower outflow boundary, following a high transmissivity channel. But, as for the particles that travel to the left, they are not entrapped by the contact area because of a relatively higher transmissivity zone inside the contact area, which allows the particles to pass through without delays. At this shear displacement, the particles that take more time travel towards the upper boundary. As mentioned in the previous paragraph, the contact area located closely to the left of the centre has some low transmissivity zones near the upper inflow boundary, which deviate a few particles to the left and entrap other few particles. Like the case of 3.0 mm shear displacement, the particles placed in the upper part of the right-hand side inflow boundary are influenced by the predominating flow perpendicular to shear direction and reach the upper outflow boundary. This tendency, as it can be seen in Figure 4.32, is maintained during the rest of the shearing process.
At 10.0 mm shear displacement, the particles that travel in the $y$-direction are clearly faster than the ones that travel in $x$-direction (parallel to shear direction). The particles that reach the lower outflow boundary of the fracture continue to be the fastest, and some particles placed in the right-hand half of the upper inflow boundary reach the upper outflow boundary with reduced time. Nevertheless, the contact area created at the left of the centre of the fracture continues to deviate particles to the left and delays some particles that start at the upper inflow boundary. At this shear displacement, as it can be seen in Figure 4.33, the number of particles reaching an outflow boundary in the $y$-direction is almost the same as the number of particles reaching an outflow boundary in the $x$-direction. This fact shows that the transport perpendicular to shear direction gains strength in front of the high transmissivity area located in the left part of the particle, which attracts the particles of its neighbourhood at the beginning of the process. As for the velocity of the particles, the 90 % of them breaks through in less than 2 seconds. The slowest particle, which reaches the left-hand side outflow boundary, takes 7 seconds, indicating that it may have been entrapped in the contact area that is located to the left of the centre of the fracture.

Finally, at 20.0 mm shear displacement, as it already happens for the case of 10.0 mm shear displacement, the particles travelling in the $y$-direction, i.e. perpendicular to shear direction, clearly travel faster than those that travel in the $x$-direction. It has to be noted that when the first particle reaches an outflow boundary in the $x$-direction, 85 % of the particles have already reached an outflow boundary in the $y$-direction. This is due to the shear induced channelling formed perpendicular to shear direction. Nevertheless, as the transmissivity field is not homogeneous and the radial flow tends to spread the particles widely, a few particles do not follow the high transmissivity channels and spend some more time. However, this delay is insignificant compared to the delay met by some of the particles that travel towards the left, as it can be seen in Figure 4.33, where the slowest particle travelling to the left takes three times the time in which the slowest particle travels in the $y$-direction. This delay in the transports towards the left of the particle is due to the contact area that is found closely to the left of the centre.

To sum up, shear induces a shift in the direction along which transport is predominant, from the $x$-direction to the $y$-direction, i.e. from parallel with the shear direction to perpendicular to the shear direction. This is due to the formation of high transmissivity channels in the direction perpendicular to shear direction, through which the particles can travel faster. Furthermore, shear produces a rapid decrease in the travel time of the particles, and though a few of them follow complex paths in order to avoid some low transmissivity areas, they are not significantly delayed.
Results and Discussion

(a)

(b)
Figure 4.33. Breakthrough curves at different shear displacements for radial flow under translational shear (a) 0.0 mm, (b) 1.0 mm, (c) 3.0 mm, (d) 5.0 mm, (e) 10.0 mm and (f) 20.0 mm shear displacement.
4.2.3.2. ROTARY SHEAR

Radial flow under rotary shear tests in laboratory are performed using cylinder specimens, because applying a torque to a rectangular specimen presents geometrical complications (Olsson, 1992; Olsson *et al.*, 1993; Cheon *et al.*, 2002). Nonetheless, the numerical modelling can be conducted to simulate rotary shear with a square rough rock fracture sample. Koyama *et al.* (2004) studied the effect that rotary shear has on radial flow for the same square sample used in this study with a rotary angle up to 90°. It has to be noted that, as explained in the methodology section, the upper part of sample size for the rotary shear is smaller than the upper part of the sample size used for the translational shear in order to guarantee a complete overlap between the upper and the lower surfaces of the fracture during the rotary shearing. Thus, the comparison of the results between the translational and the rotary shear must be qualitative, rather than quantitative.

As it has been argued in the methodology section, in this study a rotary shear up to 10 degrees is considered. Figure 4.34 shows the transmissivity distribution and the paths that particles follow at different rotation angles for radial flow undergoing rotary shear. It can be seen how the particles follow paths quite similar to those of the parallel plate fracture, as shown in Figure 4.31. Moreover, for rotary angles equal and greater than 2.0 degrees, all the particles go from its starting inflow boundaries to its corresponding outflow boundary. This can be explained because, as it can be seen in Figure 4.34, the flow pattern becomes rapidly isotropic with rotation. In addition, the transmissivity of the fracture increases significantly during the 10° rotary shear process over the whole fracture surface, except for two contact areas that are formed due to the rotation. Particle transport for radial flow during rotary shear is much more homogeneous than in the case of translational shear.

For the breakthrough curves, the arrival of the particles to each boundary as well as the directional and the general behaviour are analysed. As it can be seen in Figure 4.35, the particle transport undergoes several changes during the rotary shear process. To begin with, it has to be emphasized that the breakthrough curve at zero shear displacement is different for rotary shear from that with translational shear, due partly to the smaller sample size. Despite the fact that, as expected, for rotary shear the vast majority of the particles arrive in less time than for translational shear, because the distance is smaller, the slowest particle in the rotary shear test takes more time than that in the translational shear, maybe because it gets entrapped in a low transmissivity area. Like in the case of translational shear, the fastest particles are those that travel to the left, probably because there is still a higher transmissivity in this direction than in the others. Thus, a few particles that flow in the y-direction are deviated towards the left outflow boundary.
Figure 4.34. Transmissivity distribution and particle paths of a numerical fracture sample at different shear displacements for radial flow under rotary shear.
At the first step of rotary shear, 1.0 degree, the travel time is reduced drastically, by a 90% of the initial travel times without shear. This is due to the fact that the transmissivity field becomes very isotropic, with a significant increase in the transmissivity values, as it can be seen in Figure 4.35, due to almost uniform dilation over the whole sample area. Although the particles that travel to the left continue to be the first to reach the outflow boundary, the slowest particle also reaches this boundary. This particle is delayed in a low transmissivity area that can be seen in Figure 4.34 for 1.0 degree on the top left-hand side corner of the simulated fracture. The last particles to arrive at an outflow boundary are those that travel to the top of the fracture, with some particles being deviated towards the x-direction, reaching whether the left or the right-hand side outflow boundaries. Therefore, at the start of the shearing process, the transport in the x-direction attracts more particles than in the y-direction.

At 3.0 degrees rotary angle, as mentioned before, the particles follow a similar distribution as in the parallel plate fracture, and the same number of particles reaches every outflow boundary. In this case, the fastest particles continue to be the ones that travel to the left, but the fastest particles to reach the other outflow boundaries spend little more time. The slowest particles travel in the y-direction, maybe because of the formation of two contact areas, one in the centre near the lower outflow boundary, and the other a little distance to the right of the top left-hand side corner. As for the travel time, it is greatly reduced again and most of the particles arrive in less than 2 seconds. As for 5.0 degrees rotary angle, the particles follow a similar tendency as in the previous case. The particles start arriving at the outflow boundaries at a similar time and almost 90% of the particles arrive in less than 1 second. Again, a few particles are delayed in the y-direction, probably because the previously mentioned contact areas.

For larger rotary shear angles, the shape of the breakthrough curves becomes very similar. With 7.0 degrees of rotary angle, almost all the particles reach an outflow boundary in less than 0.6 seconds. The fastest particles are found in the top left half of the fracture, and the slowest particle travels to the upper outflow boundary of the fracture. Similarly, with 10.0 degrees of rotary shear, most of the particles travelling to the top and the left outflow boundaries of the fracture are faster than those that travel to the bottom and the right of the rough fracture. In this case, the majority of the particles arrive at the outflow boundaries in between 0.1 and 0.3 seconds, which is a result of the isotropy of the flow field of the fracture undergoing rotary shear. As it can be seen in Figure 4.34, at 10.0 degrees of rotary angle, the contact area in the low part of the fracture is very clear and has rotated a little to the right. As expected, the particles bypass around this contact area, seeking for the easiest path to continue.
Results and Discussion

(a)

(b)
Figure 4.35. Breakthrough curves at different shear displacements for radial flow under rotary shear (a) 0.0 degree, (b) 1.0 degree, (c) 3.0 degrees, (d) 5.0 degrees, (e) 7.0 degrees and (f) 10.0 degrees.
Comparing the two shearing processes for the radial flow pattern, it can be seen that the range of travel time is wider for translational shear than for rotary shear. Furthermore, unlike translational shear, in which the breakthrough curves for \( x \)-direction and \( y \)-direction are quite different in path distribution and travel time, rotary shear presents very similar breakthrough curves in all directions, both in shape and travel time. Consequently, it seems clear that while translational shear has an anisotropic transport behaviour, with faster transport in the \( y \)-direction, rotary shear presents isotropic flow field and transport paths in all directions.