Author’s response to the review suggest by anonymous Referee #2

Journal: SE
Title: Simulating stress-dependent fluid flow in a fractured core sample using real-time X-ray CT data
Authors: Kling et al.
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Dear Anonymous Referee,

We appreciate your precious time, your efforts and the very valuable comments that facilitating the improvement of the quality of the manuscript. We have addressed all concerns and recommendations indicated in the review report. On the basis of the constructive requests and hints, we suggest some corrections and reconsiderations to the manuscript that will improve the quality and consistency of our paper.

Response to Referee #2

Comment → Author’s Response → Author’s changes

Comment 1:

Page 3 lines 23-24, Page 6 lines 28-32, Page 7 lines 20-21: There is a major misconception regarding CT numbers throughout the manuscript, X-ray attenuation is a function of density and apparent atomic number (this is why contrasting agents are often employed!). The variation of the CT numbers for the sample shown is not only a function of density, but also composition. The variation of the CT numbers being a function of density and composition can have a significant effect on the estimation of the subvoxel fracture aperture.

I do not believe the methods used by the authors to extract the fracture geometry from the CT images have been properly assessed. Specifically, the effect a locally varying matrix CT number has on estimated subvoxel fracture apertures. The fracture apertures of interest are far smaller than the voxel dimensions. Therefore, as outlined by the authors, the apertures are instead estimated from the CT numbers of the voxels containing the fracture (CT(i)). To estimate the local aperture the *authors use a method that requires assumptions that may be significantly erroneous; Equations (1) and (2) summarize the MA method,*

*Local Aperture = 1/C*CT(MA)=1/C*(CT(mat)-CT(i)).*

The underlying conception of the MA method used by the authors assumes the following weighted volume average contributes to the measured CT(i),

*CT(i)=(VolumeLocalMatrix/voxelVolume)*CT(local matrix) + (VolumeWater/voxelVolume)*CT(water),*

where the voxel volume and CT(water) are constants, and CT(local matrix) is the CT number of the matrix within that voxel, CT(i). Only CT(i) is known, therefore, unless CT(local matrix) is also known, the volume of water occupying the voxel – and subsequently the estimated aperture of the fracture – cannot be determined. It is apparent from the CT image in figure 3 that the matrix CT numbers, CT(local matrix), vary locally and significantly. The authors address this issue by using a mean for CT(mat) that is varied globally in accordance with the standard deviation of the CT-number distribution of the matrix. This is the equivalent of extracting one realization of the possible fracture geometries within the framework of the method and the known uncertainties, then simply dilating (CT(mat)+standard deviation) and closing (CT(mat)-standard deviation) this geometry. To determine the variance in the simulation results as a result of local variation of the unknown CT(local matrix) would require a local analysis. A local analysis would result in a large number of possible fracture geometries that likely could vary substantially from those estimated by applying a variation in CT(mat) globally. If the objective of the investigation presented by the authors is to develop a methodology for estimating the flow path characteristics – which can conceivably range from a singular main flow path, to multi-stranded flow paths, to uniform flow – as a function of fracture geometry, which is coupled to stress history, then the local variation in aperture will be the determining factor. Bulk measurements - such as the permeability - can easily be fit by a planar plate model, therefore matching bulk measurements to simulated bulk measurements does not provide any information on the flow path geometry characterization. Likewise, if the uncertainty in the aperture variation on the local scale is large, the uncertainty of the flow path characterization will also be large, and thereby defeating the purpose of the proposed methodology. From what is presented here a rather simple conclusion may be reached, if CT(mat) varies locally and significantly then the estimated sub-voxel fracture apertures determined using the MA method may be far too uncertain to be of use in characterizing flow path geometry. Of course, this conclusion could be reached without the investigation presented by the authors. Unless the above outlined concerns are addressed the investigation presented by the authors amounts to a computational exercise that is likely disconnected from the system of interest by non-trivial uncertainty.

Response:

We partially agree and would like to thank the reviewer for pointing out this very important issue! It is right that the applied method has some limitations especially concerning the compositional issue. This important aspect misses in the introduction and discussion part.

One objective was to introduce a method that results in flow simulations that optimally reproduce the experimental results in a fast and practical way. In a prospective view, this method should provide the application of simplified equipment which only regulates confining pressures and that fracture flows can be predicted by simulations.

It is correct that $CT_{localMatrix}$ describes the most vague parameter since this value normally depends on the local composition of the matrix. So that a local (but more trivial) approach would be necessary to achieve more precise results in the case that there are significant compositional material contrasts. Our sample predominantly is composed of two minerals: Quartz and plagioclase (Weissbrod and Sneh, 2002) which, both, should have similar attenuation properties that are quite low compared to most other minerals (Ketcham, 2005) and should be represented by the chosen homogeneous CT_{mat}. It is correct, there are also brighter voxels (with $CT_i > CT_{mat}$) in the matrix that most widely can be assigned to a further alkali-feldspar component. This should cause local underestimation of apertures and should be discussed in the error analysis. Despite that, we used a modification of the original MA method (new name: MSMA → Response Referee1), also used by various authors (Johns et al., 1993;Keller et al., 1999;Keller, 1997), who also used a global CT_{mat} granting possible errors.

Nevertheless, although our sample contains compositional heterogeneities calibrated aperture seem not to be completely arbitrary which, particularly, becomes clear when comparing simulated flow paths with channels revealed by using local CT_{mat} values for a 2D view (Huo and Benson, 2015), which coincide quite well. Furthermore, compositional heterogeneities cause a loss in accuracy, however most main-channels can be reproduced, which also becomes evident due to stress related kinematics. Additionally, applying our method still provides better results than applying a simple (and also practical) parallel plate model ($k=a_h^2/12$) for the aperture data provided by the local CT_{mat} approach and, hence, still provide the better approximation of fluid flow for very small apertures (<35 µm). Although, there is a significant sensitivity to uncertainties in CT_{mat} (also provided by the heterogeneity) approximated results still are within an acceptable range. Thus, the introduced method can be described as an imperfect, but still a fast and practical prediction method, compared to other approaches, for an initial insight into fracture flow.

To address the above discussion in the manuscript, the following changes were performed:

- Page 3, lines 29-31: Detectable material contrasts can be caused by significant changes in density, such as the transition from solid to air, or composition affecting the X-ray attenuation.
- Page 4, lines 26-29: Particularly for field work, where time often plays a significant role, a functional approach without time-consuming operation procedure and costly equipment can be an asset. Thus, a method would be

necessary that only requires a fast CT scan of a pressurized dry sample to predict fluid flow under predefined boundary conditions.

- Page 5, lines 4-7: Imaging is performed by simultaneously conducting medical CT scans and core-flooding experiments allowing the validation of the simulated results.
- Page 6, lines 15-16: Additionally, the core-holder is positioned in a medical X-ray CT scanner (General Electric Hi-Speed CT/I X-ray computed tomography) to reveal real-time images of the sample for every stress stage under dry conditions.
- Page 7, lines 25-31: In this study, CT_{mat} represents a idealized global threshold value for the matrix material assuming a homogeneous rock matrix as also assigned in prvious studies (Johns et al. 1993; Keller, 1997; Keller et al., 1999). Indeed, using a global CT_{mat} is a simplified assumption and provides additional errors particularly for heterogeneous rocks (Keller et al. 1997), however is sufficient for the intended straightforward purposes of this study. Usually, heterogenous rocks would require the usage of local CT_{mat} values (e.g. Huo et al., 2016), which would result in a large number of possible solutions and would not improve the validity of the presented results.
- Page 11, lines 16-25 (also part of the response to Comment 7&8): Furthermore, additionally enhanced fluid flow is observed in single parts within the matrix (**Fehler! Verweisquelle konnte nicht gefunden werden.**). Comparing with the CT image (Figure 3) indicates that this flow occurs along laminations containing darker matrix voxels where $CT_i < CT_{mat}$ according to Eq. (3). In homogeneous media, CT_{mat} simply should represents the predominant mineral phase. In fact, the rather heterogeous sandstone in this study is dominated in quartz (detrital grains and cement), however is also enriched in feldspar. This feldspar component predominantly consists of plagioclase with minor alkali feldspars (Weissbrod and Sneh, 2002). Although, there are compositional differences, quartz and plagioclase typically reveal similar and compared to other minerals relatively low CT_i values (e.g. Ketcham, 2005; Tsuchiyama et al., 2005). Thus, the assumed CT_{mat} (1862.6 HU) can be ascribed to these dominant mineral phases. Hence, regions with significantly lower CT_i value are caused by significant porous regions. This porosity heterogeneity is also observed in thin sections (Huo et al., 2016, Huo & Benson, 2015).
- Page 14, lines 2-10: Being apparent from Figure 3, there are significant material heterogeneities within the sample. While darker voxels (with $CT_i < CT_{mat}$) can be assumed to contain more porous regions as discussed above, there are also significant brighter voxels (with $CT_i > CT_{mat}$). These significant higher CT_i (partially $CT_i > 1900$ HU) values can be ascribed to the local accumulation of alkali feldspars, typically revealing much higher CT values (up 100 HU) than quartz due to the high attenuation of potassium (Ikeda et al., 2000). Hence, locally presented alkali feldspars in a voxel can cause a local underestimation or even closing of the calibrated local aperture according to Eq. (3), most likely making a significant contribution to the underestimation of permeabilities at lower pressures (cf. Figure 7a).
- Page 14, lines 12-13: Additionally, this local underestimation can be reinforced by an inappropriate choice of the threshold value CT_{mat}, which also implies some uncertainties.

- Page 15, lines 6-7: Thus, the resolution-caused generalization of these features per voxel underestimates experimental permeabilities at lower stresses, in addition to rather prevailing compositionally caused underestimation of local apertures, due to a reduction in actual (sub-grid-scale) connectivity.
- Page 16, lines 19-28 (together with new Figure 8b instead of former Figure 8a): Additionally, Figure 8b represents a comparison of our simulations with another economical approach based on the cubic law to predict fracture permeabilities. Permeabilities are predicted empirically by applying various prominent approaches based on the mean mechanical aperture (a_m) and its standard deviation (SD) for every single pressure stage (Amadei and Illangasekare, 1994; Barton and de Quadros, 1997; Lomize, 1951; Louis, 1967; Patir and Cheng, 1978; Renshaw, 1995). The input parameters are predefined by a more precise MA approach using local CT_{mat} values and can be found in Huo & Benson (2015). As apparent from Figure 8b, the results of this alternative prediction approach reveal a wide range of possible permeabilities, which all clearly overestimate actual measured permeabilities by a minimum factor of 11 and a maximum factor of 600. These sigificant deviations result from the underlying empirical approaches that respectively are validated for different kind of fractures in various media and most widely are calibrated for relative roughnesses (SD/a_m) away from roughnesses (between 0.98 and 1.17) in this study.
- Page 16-17, lines 30ff: Accordingly, the introduced MSMA method represents a further approximating step for successful CFD simulations, but also exposes limitations. Although, applying the method with a global CT_{mat} affirm a loss in accuracy as predicted by Keller (1997) for smooth fractures (< 35 µm), however simulation results still are valuable approximates of actual permeabilities in such fractures. Indeed, in this study compositional heterogeneities provide inaccuracies as predicted by Keller (1997), however are not that dominant causing a complete loss of information as indicated by the kinematics of several reproducible flow channels. Nevertheless, inaccuracy is not only provided by compositional heterogeneities, but also by sub-grid scale features particularly regarding higher confining pressure and, thus, closing local apertures.
- Correspondingly, the abstract (page 1) and conclusion (page 18-19) were adjusted.

Comment 2:

Page 6, lines 11-12: The authors should show that five averaged scans reduces noise in comparison to a single image, how much does it reduce noise? Is it significant?

Response:

We agree, however this is extensively addressed by the cited references. Nevertheless, the following changes were performed:

- Page 6, lines 20-22: Furthermore, at each stress stage, multiple (five) scans are conducted and averaged afterwards, representing a practical method to reduce the random noise of CT scans by 50% as extensively discussed by Huo et al. (2016) and Pini et al. (2012).

Comment 3:

Page 6, lines 17-18: How is the resampling performed? Are the CT number values of the resampled voxels equal to the imaged voxel? Also do you mean one voxel to 16 voxels?

Response:

We definitely agree and performed following changes:

- Page 6, lines 26-31: After reading the five data sets, every CT scan is resampled to an isotropic voxel size (one voxel of $0.5 \times 0.5 \times 1.0$ mm³ to 16 voxels of $0.25 \times 0.25 \times 0.25$ mm³) required for a proper computation of the CFD program. Subsequently, the five scans are averaged to a single image (**Fehler! Verweisquelle konnte nicht gefunden werden.**). In a further step, geometric information stored by single CT numbers of the (resampled) voxels are transformed voxel-wise to according geometric (local apertures) and hydraulic (local permeabilities) properties being essential for the flow simulations.

Comment 4:

Figure 4: The linear calibration used was matched to known apertures (by use of spacers) that are far larger than those inferred for flow simulation, casting doubt on the extrapolation of the calibration to the apertures inferred.

Response:

We generally agree that the extrapolation of the aperture calibration can cast doubt and, therefore, is recommended for systematic studies (Page 18, lines 17-23). However, the linear relationship has been applied successfully in the cited references also using spacer calibration and is physically derived by Huo et al. (2016). To provide best possible accuracy of the calibration for every spacer four distinct slices has been chosen and MA has been considered point-by-point along the slices resulting in a total of 380 points per spacer. As discussed on page 13 (line 21-24) inaccuracy of the calibration line in the extrapolated area do not have an enormous impact on the results. Thus, the following changes were performed:

- Page 7, lines 12-16: According to that, Johns et al. (1993) suggested a calibration-based linear relationship between aperture width and the integral of the full measured anomaly which was subsequently confirmed in several fracture aperture studies (Bertels et al., 2001; Heriawan and Koike, 2015; Huo and Benson, 2015; Keller, 1997; Ketcham et al., 2010; Van Geet and Swennen, 2001; Vandersteen et al., 2003; Weerakone and Wong, 2010) and physically derived by Huo et al. (2016).
- Page 13, lines 26-30: Furthermore, in order to be valid and as introduced in Sect. 2.3, the MSMA method requires a linearity of the calibration line as reinforced by a careful calibration according to Huo et al. (2016), who also physically derived the linear relationship that justifies the extrapolation of apertures as performed here.

Comment 5:

Page 7, lines 30-32: The authors state that apertures affect 2-3 voxels, but assume only a single voxel measurement is necessary to obtain the aperture. Isn't this information loss? Wouldn't this have an effect on the estimated fracture aperture? Do the 2-3 voxels reference resampled or original image voxels?

Response:

We fully agree. This sentence was mistakably written. The following changes were therefore performed:

- Page 8, lines 13-15: Considering several cross sections through the fracture used here (before resampling) indicates that occasional local apertures affect 2-3 voxels, where the vast majority (≥ 99%) of the attenuation is captured by the central voxel causing a local but marginal information loss.

Comment 6:

Page 7, line 34: The authors state that the MA method works well. Based on what evidence?

Response:

We agree. The following changes were performed:

- Page 8, lines 19-21: However, since the model is calibrated voxel-wise, the applied method becomes increasingly inaccurate (which is also coupled to the CT resolution) with increasing fracture widths.

Comment 7 & 8:

Page 8, lines 11-13: Yes, higher porosity should reveal lower CT numbers, if the composition does not affect the CT numbers.

Page 8 lines 10-15: I am confused by this paragraph, are the authors suggesting that the CT numbers of the matrix can be used to determine the pore sizes? Given the matrix has a permeability several orders of magnitude smaller than the fracture, the flow in the matrix can be ignored. Flow in the matrix is then discussed on pg 10-11: Are the authors suggesting that there is significant flow in the matrix? The permeability assigned to the matrix using the non-sequitur method outlined on page 8 are arbitrary, CT numbers do not provide any information beyond an estimate of porosity if one assumes CT(local matrix) is known.

Response:

We partially agree. Indeed, there are compositional heterogeneities in the matrix, however major matrix is composed of quartz and plagioclase revealing similar X-ray attenuation (as discussed in the response of Comment 1). Since CT_{mat} most widely should reveal the threshold value of these minerals with a comparatively very low attenuation value, significant darker voxels in the matrix (where $CT_i < CT_{mat}$) must comprise a further phase (e.g. air) with a significant lower CT value indicating the presence of a porosity heterogeneity within the sample as also observed by thin sections. Thus, the consequent permeability anisotropy is artefact without consequences caused by the sample, but can supportive for issues cited below. Since there are no validation experiments for fracture-matrix-interaction this conclusion was overachieving but should be considered in future studies. Based on that, the following changes were performed:

- Page 8, lines 28-31: Although, this strategy does not describe the basic intention of the common MA method, it provides a convenient solution to include data for the entire core and also enables integrations of regions with higher porosity within a homogenous matrix material where fluid inclusions should decrease CT_{mat}. Hence, voxels representing sections of the matrix with significant porosity should reveal lower CT numbers ($CT_i < CT_{mat}$) so that these voxels, in simplified terms, are treated as equivalent apertures.
- Page 11-12, lines 16-3: Furthermore, additionally enhanced fluid flow is observed in single parts within the matrix (**Fehler! Verweisquelle konnte nicht gefunden werden.**). Comparing with the CT image (Figure 3) indicates that this flow occurs along laminations containing darker matrix voxels with $CT_i < CT_{mat}$ according to Eq. (3). In homogeneous media, CT_{mat} simply should represent the predominant mineral phase. In fact, the rather heterogeous sandstone in this study is dominated in quartz (detrital grains and cement), however is also enriched in feldspar. This feldspar component predominantly consists of plagioclase with minor alkali feldspars (Weissbrod and Sneh, 2002). Although, there are compositional differences, quartz and plagioclase typically reveal similar and, compared

to most other minerals, relatively low CT_i values (Ketcham, 2005; Tsuchiyama et al., 2005). Thus, the assumed CT_{mat} (1862.6 HU) most widely can be ascribed to these dominant mineral phases. Therefore, regions with significantly lower CT_i values are caused by significant porous regions. This porosity heterogeneity is also observed in thin sections (Huo et al., 2016, Huo & Benson, 2015). However, the simulated overall matrix permeability can be assumed to be rather low which is also clarified by carefully examining the propagation of the pressure fields corresponding to the predefined bulk matrix permeability of 10^{-19} m². Concurrently, propagation of the pressure fields also reinforces the assumption that major fluid flow occurs along the fracture. Furthermore, comparing absolute changes in fluid flow (**Fehler! Verweisquelle konnte nicht gefunden werden.**) due to loading between the lowest (0.7 MPa) and the highest (22.1 MPa) pressure stage indicates that most changes within the sample occur along the fracture plane while the simulated matrix flow remains nearly equal. Unfortunately, core permeability is derived by solving the Navier-Stokes-Brinkman equation for the measured pressure drop over the entire sample (as stated in Sect. 2.4) which prevents the quantification of the matrix permeability. Due to the missing appropriate validation experiments and the non-significant simulated matrix flow, possible fracture-matrix interaction are not further discussed in this study and can be considered as unifluential artefacts of the matrix material. Nevertheless, the MSMA method can provide a promissing approach to simulate such issues especially considering laminated sandstone as experimentally investigated in the past (Clavaud et al., 2008; Grader et al., 2013; Karpyn et al., 2009). Indeed, this method can be errorneous for heterogeous rocks such as granite, however Watanabe et al. (2011) found that locally resulting "non-zero apertures" only have little impact on the simualtions.

- The possible detection of fracture-matrix-interaction were deleted from the abstract and conclussions.

Comment 9:

Page 12 lines 31-32: The authors state that "significant material heterogeneities appear to be negligible for the sandstone," which does not follow from the discussion on the significant variation in permeability that the simulations predict with small global changes in CT(mat). This is the opposite of negligible. Page 13 lines 9-10, the authors state that the simulations are unable to reproduce the measured permeability hysteresis. This statement certainly follows from the results, and indicates major issues with the practicality of the proposed methodology.

Response:

We agree. Please refer to the comments above (Comment 1).

Comment 10:

Page 12 line 13: The authors state, "one may assume stress-dependency of CT(mat)", why? The densities might change slightly due to compression, but the strain is likely to be very small, and the resulting effect on CT number is likely to be indiscernible.

Response:

We agree. This paragraph can be condensed. The following changes were performed:

- Page 14, lines 25-27: Indeed, the simulations can be fitted by varying CT_{mat} within the mentioned range, however the compression and resulting strain on the fine-grained sample as well as the evaluation of the single images do not endorse such a proposal.

Comment 11:

Page 14-15 bulleted recommendations: None of these recommendations follow from the study outlined in the manuscript, instead they are generalized advice that may be useful, but is disconnected from the study. For instance, bulleted point 1, I agree pore-scale studies of heterogeneous porous rocks may be valuable, but this was in no way investigated in this manuscript. Again, bulleted point 2, I agree to better understand the effect matrix permeability has on fluid flow in fractured porous rock one may want to measure the matrix permeability before inducing a fracture, I don't think anyone would disagree. And, yes it would better to have higher resolution measurements of fracture roughness and aperture distribution.

Response:

We partially agree. However, using medical CTs for numerical fracture flow studies still is an emerging method in geosciences and significantly requires systematic investigations to further medical CT as a valuable technique for similar issues. Thus, we recommend in this study a mixture of first- and second-hand experiences to provide a good starting point for future studies using medical CTs. We consider this special issue as an appropriate platform to offer these recommendations as a kind of tutorial. Nevertheless, we shorten this part in the conclusions:

- Page 19, lines 26-28: Considering the aforementioned comparative study a list of recommendations for future research is compiled, including a systematic investigation concerning different model and experimental setups, rock types, fracture modes as well as validation techniques.

In our opinion, the introduced method indeed can be described as a imperfect, however fast and practical prediction method, compared to other approaches, to approximate fluid flow even in very small fractures. Several lessons have been learned for future studies combining medical CTs data and numerical simulations regarding experimental techniques as well as mineralogical affectations. On the other hand, the paper also reveals current limitations that should be comprehensively addressed in future studies. Nevertheless, we think that the concerns of the reviewer were very valuable to improve the quality of the discussion of the simulation results. We are very thankful for that and think the anonymous referee is worth mentioning in the acknowledgements of the article.

Johns, R. A., Steude, J. S., Castanier, L. M., and Roberts, P. V.: Nondestructive measurements of fracture aperture in crystalline rock cores using X ray computed tomography, Journal of Geophysical Research: Solid Earth, 98, 1889-1900, doi:10.1029/92jb02298, 1993.

Keller, A. A.: High resolution cat imaging of fractures in consolidated materials, International Journal of Rock Mechanics and Mining Sciences, 34, 155.e151-155.e116, doi:10.1016/S1365-1609(97)00181-0, 1997.

Keller, A. A., Roberts, P. V., and Blunt, M. J.: Effect of fracture aperture variations on the dispersion of contaminants, Water Resources Research, 35, 55-63, 10.1029/1998wr900041, 1999.

Ketcham, R. A.: Three-dimensional grain fabric measurements using high-resolution X-ray computed tomography, Journal of Structural Geology, 27, 1217-1228, doi:10.1016/j.jsg.2005.02.006, 2005.

Weissbrod, T., and Sneh, A.: Sedimentology and paleogeography of the Late Precambrian-Early Cambrian arkosic and conglomeratic facies in the northern margins of the Arabo-Nubian Shield, Bulletin (Makhon ha-ge’ologi (Israel)), no. 87. , Geological Survey of Israel, Jerusalem, 2002.