# Deep learning 3D-mineral liberation analysis with micro-X-ray fluorescence, micro-computed tomography, and deep learning segmentation

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Backgrounds
Mineral liberation has become a key step in the mineral processing industry to quantitatively determine the volume fraction of valuable commodities. Several semi-automated techniques, such as backscattered electron (BSE) images with energy-dispersive spectroscopy (EDS) marketed as commercial systems such as QEMSCAN have been developed for this purpose. However, the extrapolation of the collected 2D data to 3D volumetric remains problematic. Recent developments in X-ray microcomputed tomography (μCT) made it possible to non-destructively characterise these minerals. The problem is the densities of some geomaterials are similar, hence without additional information, it is difficult and often impossible to reliably differentiate the phases just based on μCT data. In this study, we combined the micro-X-ray fluorescence (μXRF) with μCT data and develop a workflow incorporating statistical analysis and deep learning segmentation to interpolate the 2D data into 3D volume (Deep-XFCT).

Methods
The rock used in this study was a fine-grained 24 mm basaltic andesite sample that has a clear and distinct mineral inclusion. A combination of analytical techniques was used for the mineral analysis, which include (1) XRD on powder sample to understand the mineral presence and their abundance, (2) μCT to get 3D volumetric data, (3) μXRF to get elemental mapping for the mineral labels and atomic mass percentages of discrete points for mineral verifications, (4) Raman Spectroscopy to cross check the mineral identifications through μXRF data. The data processing was performed in two steps: (1) establishing ground truth labelling of the mineral phases through μXRF elemental mapping using K-mean clustering, (2) use of the ground truth labelling to train a deep learning model that will segment the mineral phases in 3D μCT data with a specific convolutional neural network architecture specifically designed for image segmentation (U-Net model) using two commercial software Dragonfly ORS and Avizo.

Results
The XRD results provided three prerequisite information for the workflow. First, the mineral phases that exist within the sample that holds important elemental information to correlate with the μXRF data. Second, the number of mineral phases that was presence, which guided the number of clusters for the K-mean clustering. Third, the mineral phases percentage abundance which were used as the validation for the cross-referencing with the K-means clustering abundances and the accuracy of segmentation from the deep learning.
The XRD shows the presence of albite, ankerite, clinochlore, illite, laumontite and quartz. By applying the geochemical principles to the K-means clustering centroids of the μXRF maps, illite, ankerite, and clinochlore can be unambiguously identified through the highest elements concentration present in each mineral. Quartz and albite were identified through the μXRF point analysis by the highest Si and Na mass percentage, respectively. Laumontite did not

have a unique elemental identifier nor characteristic combination of elements and was identified by deduction as the final element. Raman Spectroscopy was able to confirm the presence of albite, clinochlore and quartz.

The minerals assigned to each pixel of the µCT orthoslice on the top and bottom surface of the sample where a U-Net neural network model was trained to segment the µCT based on the mineral labels. From visual analysis, the model captured the major contours of the mineral phases. This includes separating the albite and illite matrix to a good approximation, despite their identical grayscale value. However, the model failed to recognise the finer details apparent in the labelled training data. The overall accuracy from all minerals for top and bottom surfaces from the U-Net model in Dragonfly ORS 2021.2 were 70.23% and 69.56%, respectively. Furthermore, the results from the U-Net model in Avizo 2021.1 were similar with 73.57% and 72.08% for the top and the bottom surfaces. To validate the segmentation from the model, the sample was cut 5mm from the top and bottom of the plug and the surfaces were subsequently mapped with µXRF to allow the mineral phases maps within the volume of the sample to be compared. In comparison to the training data, the validation data has lower but serviceable accuracy. Using the phase identification as labels, a neural network was successfully trained to segment other slices throughout the volume to obtain a 3D representation of the mineral phases in the sample.

Conclusions
Our results successfully demonstrate semi-automated multi-modal analysis with an approach that is universal to any multi-instrument approach. The blend of µXRF and µCT provides a unique opportunity for robust 3D mineral liberation analysis in both field and laboratory applications when combined with Deep-XFCT. While Deep-XFCT did not provide pixel-level accurate segmentation, it was able to provide an excellent proxy for the purposes of obtaining the presence, location, distribution, and morphology of grains dispersed throughout a core plug. It was also shown that Deep-XFCT was able to differentiate fine-grained minerals of similar density that would be impossible by manual segmentation. This technique is a valuable technique that has the potential to expedite 3D mineral liberation analysis.

**Keywords:**

Deep learning, Image analysis, Multi-modal