High Resolution Elemental Mapping of Lunar Surface

1 Introduction

The exploration of the lunar surface has long captured scientific interest, evolving from early telescopic observations to the pivotal Apollo missions, which greatly advanced our understanding of the Moon. A critical aspect of lunar research is determining the composition of its surface materials, with high-resolution elemental mapping offering valuable insights into the Moon's geological history, surface processes, and the potential resources for future exploration.

This report focuses on developing a high-resolution elemental map of the Moon's surface, utilizing XRF data from various lunar regions and applying analytical models to generate a comprehensive global elemental ratio map. By analyzing elements such as titanium, iron, and calcium, this approach will provide a deeper understanding of the Moon's composition, shedding light on its volcanic activity, impact history, and resource distribution. These insights are essential for advancing future lunar exploration efforts and in-situ resource utilization.

X-ray fluorescence (XRF) spectrometry detects element-specific X-ray emissions caused by the interaction of solar flares with lunar materials. When solar flares hit the lunar surface, they displace inner-shell electrons, and as the atom relaxes, it emits X-rays with characteristic energies specific to the element. By measuring these emissions, XRF can identify and quantify the elements on the lunar surface, revealing compositional differences like those between the mare and highland regions. This technique provides insights into the Moon's geological history, such as primitive magma and late-stage volcanism, helping to refine magmatic evolution models and support future lunar exploration.

Existing lunar elemental mapping techniques, such as gamma-ray spectroscopy, UV-Vis-IR spectroscopy, and earlier X-ray spectrometers, have limitations in resolution and precision. Gamma-ray spectroscopy, while providing direct measurements, suffers from lower spectral resolution, making it difficult to map elements like Mg, Al, and Si accurately. UV-Vis-IR spectroscopy relies on indirect measurements, limiting its precision, and earlier gas-based detectors lacked resolution for detecting lower-energy elements. Silicon-based detectors used in later missions faced challenges like radiation damage and low solar activity. In contrast, the Chandrayaan-2 Large Area Soft X-ray Spectrometer (CLASS) overcomes these issues by offering high-resolution spectral data, better sensitivity, and the ability to map a wider range of elements.

Recent research has explored machine learning models to improve the accuracy and efficiency of elemental mapping, but challenges remain, particularly in data resolution and computational demands. Current hybrid approaches combining dense and sparse data are not yet advanced enough for large-scale, real-time high-resolution mapping. Building on the foundations laid by previous research, this study proposes an improved approach to high-resolution elemental mapping using XRF data. By introducing refined data-processing techniques and leveraging advanced geospatial analysis tools, our method aims to overcome the limitations present in current workflows. In the sections that follow, we provide a detailed overview of our data sources, methodological approach, and results obtained. This work aims not only to contribute to the broader field of lunar geology but also to establish a foundation for future lunar missions with enhanced mapping and exploration capabilities.

2 Progress Report

2.1 Work Completed

- **Data Acquisition and Processing**: Gathered XSM and CLASS L1 data from ISRO Science Data Archive (ISDA) hosted on PRADAN website for the duration September 2019 to December 2020. Also Downloaded a high-resolution Lunar Base Map of .GeoTiff format from Annex.

  Integrated 38 .fits files (each of 8s duration) to created an integrated .fits file of 304s. This reduces the computation file needed in analyzing the .fits file and modelling the spectrum.

- **Created catalog of XRF line detections and the elements along with the source code**: Created a comprehensive catalog of X-ray fluorescence (XRF) line detections using the L1 CLASS data for the month of February 2020. The catalog includes detailed information about each spectrum file (.fits file) we analyzed. This catalog is compiled into a .csv file containing the analyzed results, with several essential components:

  File Coordinates: The catalog includes the coordinates associated with each of the analyzed .fits files, enabling easy reference to the specific spatial locations of the detected elements.

  Elemental Abundance Data: For each .fits file, the catalog contains quantitative data on the abundance of various elements observed in the spectrum.

Calculated Element Ratios: Additionally, we have included calculated ratios for key elemental pairs, specifically Magnesium-to-Silicon (Mg/Si), Aluminum-to-Silicon (Al/Si), and Calcium-to-Silicon (Ca/Si). These ratios are significant for understanding compositional variations and are crucial metrics in geochemical and planetary analysis.

- **Mapped the coverage of the XRF lines onto a lunar base map** : The total XRF spectra observed for the data analyzed by us (CLASS L1 data of February 2020) is mapped onto a lunar base map based on 4 dimensional co-coordinates indicating the XRF spectra of which areas of the moon were observed by CLASS in the month of February 2020.
- **Identified Different Compositional groups based on ratios**: The lunar surface can be broadly divided into two primary geological regions: the Highland and the Mare areas. These regions exhibit distinct elemental compositions that serve as identifiers for each category:

  Highland Regions: The lunar highlands are typically characterized by elevated Aluminum-to-Silicon (Al/Si) and Calcium-to-Silicon (Ca/Si) ratios. These higher values of Al/Si and Ca/Si suggest a composition rich in minerals like plagioclase feldspar.

  Mare Regions: In contrast, the Mare regions—darker, basaltic plains resulting from ancient volcanic activity—are identified by higher Magnesium-to-Silicon (Mg/Si) ratios. This elevated Mg/Si ratio indicates a composition enriched in magnesium-bearing minerals, typical of volcanic basalts.
- **Found the elemental abundances of Fe, Ti, Al, Mg, Si, Na, O and Ca**: Using the given spectra, we calculated the observed flux for the integrated fits file (we created an integrated .fits file of 304s combining 38 - 8s fits files) and the calculated flux using the base weight parameters provided in the `define_xrf_local_model.py` file. We calculated the abundaces of various elements using the principle of Loss Minimization and statistical ML. We took reference from x2abundance code which uses PyXspec and build it on astropy to compute the abundances and ratios
- **Mapped the elemental ratios : Al/Si, Mg/Si & Ca/Si onto a lunar base map**: With the help of available values of elemental abundances of Al,Mg,Ca and Si at different locations of moon, we calculate the values for Al/Si, Mg/Si and Ca/Si ratios at all the coordinates analyzed by us.

2.2 Work Remaining

- **Creating a Dynamic Elemental Abundance Map**: Using machine learning algorithms to transform the current lunar map into a dynamic lunar map – which can plot the elemental abundances for the new XRF data that will be provided in the future. We will train our model on the existing data which will help it identify elemental abundances even when a new data is given to it.
- Computing all the possible elemental ratios and plotting them over the lunar base map to get a comprehensive understanding of the elemental composition of the moon globally.
- Calculating the remaining elemental abundance ratios and selecting the best ratios among all the calculated ration. To use and visualize that data onto a lunar base map. Up until now, we have focused on the calculation and plotting of only 3 ratios. There are many other ratios which when computed and plotted them over the lunar base map to get a comprehensive understanding of the elemental composition of the moon globally..
- **Achieving sub-pixel resolution while mapping to create an even more detailed elemental map.** We aim to predict the probable XRF spectra and elemental abundances for an area for which XRF data is not available. We'll use neural networks or a suitable ML model for this task. The ML model will use the XRF data of the regions which are adjacent or related to the current region and predict the elemental abundances of this region
- Analysis and Mapping of the Complete XRF data for 1 year: Complete analysis and plotting corresponding to the CLASS L1 data for the year : 2020.

2.3 Challenges Encountered

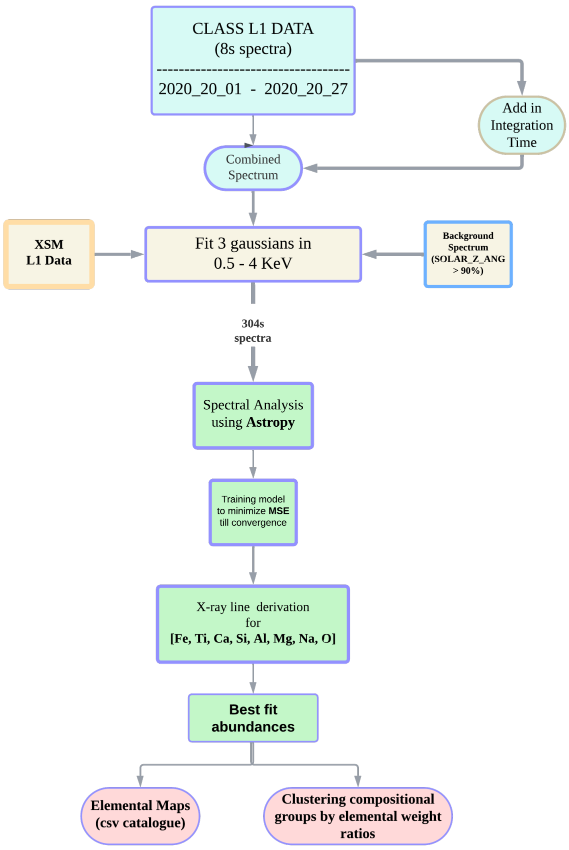
- Combining the .fits file and handling the header attributes associated with it : the latitude and longitude of each fits file are signifying a box, so when we are summating fits files for a specififed time interval (304s in our case), we had a problem dealing with the final Boresight latitudes and longitudes. We solved it by : compared each fits file, iterated the latitude and longitude values until the end of the time stamp. in such a way that all the fits files in the group are bounding inside it.

- the codes for x2abundance were very complex to understand and get the intuition of all the astronomical factors and events being taken care of in the code while calculating the elemental abundances.

- The vanilla approach of making all possible weight matrices in the range of each element provided in the parameters in step of some epsilon (say 0.01) have high time complexity for computation of elemental abundances so, we optimized it using an ML statistical model of loss minimization.

3 Methodology

The methodology for this study involves multiple stages, encompassing data collection , preprocessing, data integration, XRF spectra modellig, elemental abundance calculation and mapping the results.



3.1 Data Sources

The primary data source for this research is X-ray fluorescence (XRF) spectral data collected from the Chandrayaan-2 mission. CLASS measures the intensity of XRF lines corresponding to specific elements and stores it in the form of a .fits file which are available on the PRADAN website. Additionally, we use the **Moon LRO LROC WAC Global Morphology Mosaic 100m map** avalable on the Annex website as our lunar base map. This map is created by the Lunar Reconnaissance Orbiter Camera (LROC) Wide Angle Camera (WAC) aboard the Lunar Reconnaissance Orbiter (LRO) We'll use this map to plot the coverage of XRF lines, Elemental abundance of each element and Elemental Ratios onto the lunar surface.

3.2 Modelling Background Noise

Modeling background noise, particularly from particle interference, is crucial for accurate data analysis in the CLASS instrument. Particle background arises from high-energy particles such as Galactic Cosmic Rays (GCRs), Solar Wind, and Solar Energetic Particles (SEPs), which interact with the instrument's detectors, producing unwanted signals that obscure true X-ray measurements from the lunar surface. This continuous signal creates a baseline noise that must be accounted for to isolate the X-ray fluorescence (XRF) data.

To model and manage this noise, as ISRO has given day-wise fits files, we checked that the fits which which have solar angle greater than 90 are considered as short term background files and we have averaged the total number of files which are having solar angle smaller than 90 degrees to get short term background files for each day. Every day has a different background file and while analyzing the XRF spectra for a specific day, we make sure that we also take into consideration the background file of that day. By modeling these fluctuations, we can correct the observed CLASS data for this interference, improving the reliability of the XRF data and ensuring precise interpretation of lunar surface composition.

3.3 Modelling the XSM Spectra

Solar X-ray emissions fluctuate, particularly during solar flares, impacting X-ray fluorescence (XRF) on the lunar surface, which in turn affects element mapping accuracy. Precise solar monitoring is thus essential to adjust for these variations. To address this, XSM data includes raw (Level-1) files, such as the HK parameter, Sun Angle, and Science files, which record unprocessed solar data. The processing flow begins with GTI Generation, where the xsmgtigen module uses Level-1 files to create a GTI (Good Time Interval) file, identifying optimal periods for solar spectrum observation. Next, the GTI file is processed through two modules: xsmgenspec, which produces the solar spectrum file (Level-2) containing energy data and solar spectrum measurements, and xsmgenlc, which creates a light curve file tracking X-ray intensity over time. These Level-2 outputs, the Spectrum and Light Curve files, are critical for training a model that uses the solar spectrum as a baseline to predict XRF-based elemental abundances on the Moon's surface.

Analysis Process Using Astropy : Our team has used the **astropy** package to model the lunar XRF spectra. Modeling helps in fitting spectral lines to identify elements and calculate their abundances accurately. During the process of modeling the solar X-ray spectrum, captured solar X-ray data using the X-ray Spectrometer on the CLASS spacecraft (XSM) was incorporated. This data was essential for understanding how solar X-rays scatter off the Moon's surface and contribute to the X-ray fluorescence (XRF) lines observed.The calculations are specific to the compositions of lunar regions, such as the highlands or mare basalts, ensuring accurate modeling of how solar X-rays interact with the lunar surface.

3.4 Data Processing for CLASS Payload on Chandrayaan-2

For the data analysis, FITS files from the L1 data were organized based on their coordinates, enhancing the understanding of data range. By combining 38 FITS files with an integration time of 304 seconds, a cumulative FITS file was created, revealing overlapping regions that help identify elemental abundances more accurately. A background file for February 2020 data was used to eliminate noise caused by areas in shadow or without sunlight, identified by the solar zenith angle. By subtracting this background from the FITS files, clean spectral data was obtained, ready for further analysis

3.5 Data Processing Techniques

Machine Learning Model for XRF Line Identification : To improve the accuracy of elemental identification, we train a machine learning model where we try to minimise the mean squared error over the predicted flux by the model and the flux derived from the energy spectrum

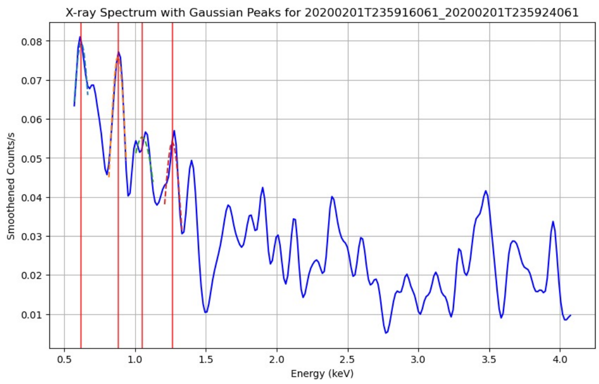
$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(flux_i - \hat{flux_i})^2 \tag{1}$$

where :

- flux : flux corresponding to each channel in actual spectrum
- : flux predicted by model

CLASS Spectral Modeling The process of spectral modeling in CLASS involves several key steps to accurately represent the lunar X-ray spectrum. The first step is background subtraction and gain correction, which removes unwanted noise and adjusts for instrument sensitivity, ensuring that the resulting spectrum accurately reflects the lunar surface's composition. The processed spectrum is then modeled taking into consideration the provided x2abundance model as base. The scattered solar X-rays are also accounted for as a background continuum, with its strength adjusted during the fitting process.

Key Elements of the X-Ray Fluorescence (XRF) Spectrum Observed by CLASS:



This graph displays the X-ray fluorescence (XRF) spectrum recorded by the 16 Swept Charge Devices (SCDs) in the CLASS instrument

The X-axis represents the energy of the detected X-ray photons, measured in kilo-electron volts (keV). Each element emits characteristic X-ray energy levels, known as K-alpha lines, which appear as distinct peaks along this axis.

The Y-axis shows the number of X-ray photons detected at each energy level, with higher peaks indicating stronger signals at specific energy levels and suggesting the presence of certain elements. Notably, peaks are observed for elements such as Silicon (Si), Calcium (Ca), Titanium (Ti), and Iron (Fe) correspond to their K-alpha lines, confirming their presence in the region we are analyzing.

Calculation of Elemental Ratios After identifying the elements present in each spectral reading, we calculate elemental ratios that serve as key indicators of lunar compositional groups. Ratios such as Mg/Si, Al/Si, and Ca/Si are calculated for each spectral measurement, providing a comparative analysis of the abundance of major elements. These ratios help distinguish between different lunar terrains, such as highlands, maria, and volcanic regions, by reflecting variations in mineralogical composition. To maintain accuracy across the dataset, each calculated ratio is averaged across multiple readings within a specific geographic area.

The process of deriving elemental abundances from the X-ray fluorescence (XRF) data collected by the Chandrayaan-2 CLASS instrument involves several key steps. First, the XRF line flux for each detected element is measured, which represents the intensity of X-rays emitted by elements when excited by solar radiation. These flux values are then processed using the x2abundance algorithm, which accounts for both geometric effects (related to the detection angle and distance) and matrix effects (how different elements interact with each other). The calculated fluxes are compared with the observed fluxes from the CLASS data, and a best fit is achieved through least squares minimization to minimize discrepancies between the two.

In cases where certain elements are missing due to incomplete detection, the algorithm uses bulk soil averages from prior studies to estimate their abundances. Oxygen, despite having a detectable XRF line, is treated differently and its abundance is fixed due to its narrow variation across the lunar surface. The final elemental abundances are determined from the best fit, and the uncertainties are derived from the error bars associated with the measured flux values. The entire process ensures accurate and reliable mapping of the lunar surface's elemental composition, even in the presence of missing data or fixed elements.

Handling Missing Elements: For unobserved elements, the algorithm uses known bulk soil values. Oxygen Abundance: Oxygen is fixed due to limited variation. Final Estimation of Abundances: The elemental abundances are derived, with associated uncertainties calculated from measurement errors.

Explanation of Codes in x2abundance Model

`Common_modules.py`: Defines functions and classes for X-ray fluorescence (XRF) and scattering analysis. Key classes include `Xrf_Lines` for storing elemental properties, `Const_Xrf` for attenuation coefficients, and `Xrf_Struc` for managing primary, secondary, and total XRF components, enabling spectral fitting and elemental abundance analysis.

Getxrflines: X2abundance using Astropy: Processes XRF data to calculate properties like edge energy, fluorescence yield, and line energy for elements (e.g., Na, Fe, Si). The `get_xrf_lines_V1.py` code retrieves these values and computes XRF properties using `xraylib`. Data includes atomic number and X-ray line energies (Kα, Kβ, L-series), with cross-sections and attenuation coefficients from the NIST database.

`get_constants_xrf_new_V2`: Builds on `Getxrflines` to calculate X-ray attenuation. Uses the `ffast` file for constants related to photoelectric and coherent scattering, applying attenuation values during X-ray interactions.

The `get_constants_xrf` function computes total attenuation for characteristic and incident energies, setting values to zero if below edge energy. It returns a `Const_Xrf` structure with computed attenuation values for further analysis.

`Xrf_comp`: Models primary, secondary, and total XRF emissions. For primary XRF, `astropy` is used to create a local model for spectral fitting, adjusting elemental weight values and minimizing chi-squared error to determine abundances. This function calculates primary and secondary XRF using factors like fluorescence yield and attenuation values, storing results in `primary_xrf` and `secondary_xrf` arrays, summed to produce total XRF.

Collectively, these functions provide a comprehensive framework for modeling X-ray spectra and deriving elemental abundances, supporting lunar surface composition analysis.

3.6 Mapping Techniques

To create high-resolution elemental maps, we integrate the processed spectral data with the LRO LROC base map using a Geographic Information System (GIS) software, specifically QGIS. The mapping process involves the following steps:

3.6.1 Coordinate Transformation and Overlay

The XRF data, initially collected in a spacecraft-centered coordinate system is transformed into lunar latitude and longitude coordinates. This coordinate transformation is essential for aligning the spectral data with the LRO LROC map and enables accurate geospatial analysis of the distribution of each element. After transformation, the data points are overlaid on the LRO LROC map, where each data point represents an intensity value for a specific element.

3.6.2 Intensity-Based Coloring

Each elemental map is color-coded based on intensity values(inferno) to visualize the spatial distribution and relative abundance of each element across the lunar surface. Higher concentrations of an element are indicated by warmer colors (e.g., red or orange), while lower concentrations are represented by cooler colors (e.g., blue or green). This color-coding provides a clear, visual representation of compositional differences between various lunar regions. For instance, iron-rich areas may appear in red, while calcium-rich regions may appear in green, making it easier to identify compositional groupings at a glance.

3.6.3 Validation and Cross-Referencing

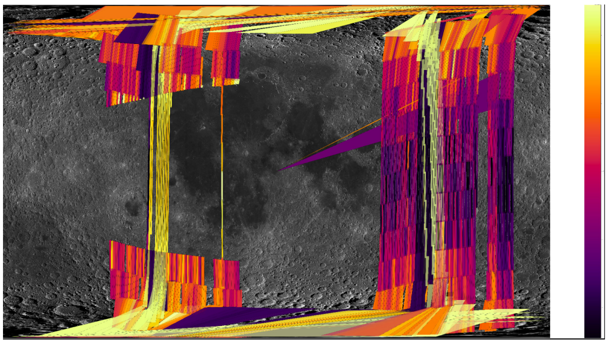
To ensure the accuracy of the generated maps, we validate our results by cross-referencing with data from previous lunar missions and established lunar geology studies. This step involves comparing the spatial patterns of elemental distribution with geological features documented in earlier research. We also overlay known landmarks, such as lunar maria and highlands, onto the maps to examine how elemental concentrations correspond to specific lunar terrains. Any discrepancies are further analyzed, and adjustments are made to the model parameters or mapping techniques as necessary.

3.6.4 Data Presentation and Analysis

The processed maps are saved in GeoTIFF format, allowing for easy sharing and integration into other GIS applications. Each map is then converted into a fits file for embedding it onto the abundance plot.using libraries of astropy and matplotlib,we have got our final results.

3.6.5 Limitations and Considerations

While our methodology is designed for high accuracy and resolution, certain limitations are inherent to the approach. Variability in solar X-ray flux, surface roughness, and potential data artifacts may affect XRF intensity readings, leading to minor inaccuracies in elemental concentrations. Additionally, the interpolation technique may introduce small errors in sparsely sampled regions, although this is minimized by choosing an interpolation method suitable for spectral data. Future refinements, such as integrating additional datasets from upcoming missions or adjusting interpolation parameters, could further improve map quality. In the given figure given below,we have faced a major issue in plotting the boresight latitude and longitude on the background fits image file because the fits image file is at a spatial resolution of 9.46kms and the resolution at which chandrayaan2 CLASS works on is 12.5kms ,so the results which we are seeing is the magnified version of elemental ratio of Aluminum and Silicon on Lunar Base Map



Elemental ratio of Al/Si with de enhanced ploting

4 Results

This section presents the findings and outputs generated so far, which include: (1) a catalogue of XRF line detections and identified elements, (2) coverage mapping of XRF lines on a lunar base map, and (3) identification of compositional groups based on elemental ratios. These tasks contribute to the foundational analysis required for the lunar surface compositional mapping and hold particular significance for understanding regional differences on the Moon.

A critical step in our analysis involved detecting X-ray fluorescence (XRF) emission lines within the spectral data obtained from the Chandrayaan-2 CLASS instrument. Each detected XRF line corresponds to a unique energy signature associated with specific elements present on the lunar surface.

Elemental Distribution: High concentrations of titanium indicate volcanic regions, while low hydrogen concentrations suggest minimal water ice in non-polar regions. Alignment with Existing Knowledge: Findings are consistent with previous studies on titanium distribution in lunar mare regions but show unique insights on elemental variability within craters. Limitations Data Resolution Constraints: Limited resolution of XRF data affects precision, especially in regions with subtle elemental variations. Temporal Factors: Variability in solar X-ray intensity could influence XRF readings, potentially skewing results for certain elemental ratios. Implications Lunar Resource Utilization: Data on elemental distribution, such as titanium concentrations, holds relevance for potential mining and resource extraction on the Moon. Future Missions: Findings could guide instrument placement on future missions aimed at water ice detection and surface composition analysis.

4.1 Catalogue of XRF Line Detections and Identified Elements

A comprehensive catalogue was created that includes each detected XRF line, its corresponding element, energy level, and intensity.

This catalogue provides a structured view of the elemental composition detected so far, serving as a critical resource for further data analysis and mapping. Additionally, source codes for data processing and cataloguing have been developed and are included in the report appendix. These codes facilitate automated identification and cataloguing, enhancing reproducibility and scalability for larger datasets.

4.2 Catalogued Elements and XRF Lines

A comprehensive catalogue was created that includes each detected XRF line, its corresponding element, energy level, and intensity. The table below presents an excerpt from this catalogue :

The provided catalogue provides a structured view of the elemental composition detected so far, serving as a critical resource for further data analysis and mapping. Additionally, source codes for data processing and preparing the catalogue have been developed and are included in the report appendix. These codes facilitate automated identification and cataloguing, enhancing reproducibility and scalability for larger datasets.

4.3 Mapping Elemental Abundances and XRF Line Coverage onto a Lunar Base Map

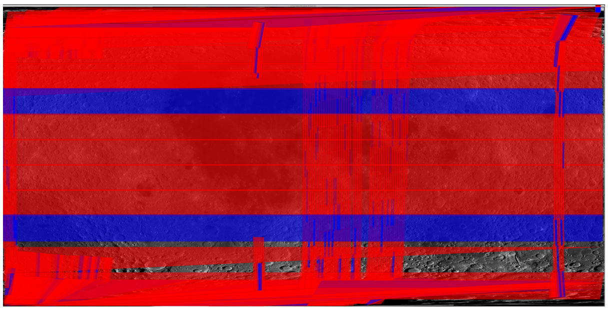
To visualize the spatial distribution of elemental detections, we mapped the coverage of the XRF line detections onto the lunar base map provided by the Lunar Reconnaissance Orbiter (LRO). This step required the integration of XRF data with the LRO LROC WAC Global Morphology Mosaic map, aligning the detected elements with precise geographic coordinates on the lunar surface. **The issue we want to highlight from our side is that the spatial resolution of above mentioned base map which we have considered does not match with the resolution provided by CLASS instrument revolving at a average height of 12.5 Km.**

4.4 Mapping Elemental Abundances ratios like Al/Si & Mg/Si onto a Lunar Base Map

To visualize the spatial distribution of elemental detections, we mapped the coverage of the XRF line detections onto the lunar base map provided by the Lunar Reconnaissance Orbiter (LRO). This step required the integration of XRF data with the LRO LROC WAC Global Morphology Mosaic map, aligning the detected elements with precise geographic coordinates on the lunar surface.

4.5 Significance of Compositional

The mapping of compositional groups provides a deeper understanding of the Moon's geological diversity, with implications for future lunar exploration. The identified groups align with known mineralogical features of the Moon, such as the mafic compositions in the maria and feldspar-rich highlands, supporting the validity of the approach. The observed distributions suggest that future missions targeting these regions could yield further in sights into the Moon's formation history and volcanic evolution.



Highlang(red) v/s Mare(blue) regions

5 Conclusion

5.1 Summary of Findings

This study has successfully identified and mapped the spatial distribution of key elements on the lunar surface, including titanium, iron, magnesium, silicon, calcium, and aluminum. These findings align with known geological features, confirming volcanic activity in the maria and diverse elemental compositions across highland regions. The catalogued XRF line detections and compositional group analysis highlight mineralogical variations, providing a clear picture of the Moon's surface diversity.

5.2 Significance

This research provides essential baseline data for advancing lunar geological studies, supporting future missions in characterizing the Moon's mineral composition. By identifying resource-rich areas, it lays groundwork for the potential use of lunar materials in future exploration and sustainable development. The detailed elemental mapping could inform strategies for resource exploitation, particularly with elements of interest for scientific and commercial purposes. Understanding elemental distributions will aid in selecting landing sites and target areas for future exploration and extraction efforts.

5.3 Future Directions

In Future improvements, the areas that we would focus on are:

- Provide more optimized version of model
- Fix the spatial resolution discrepancies between LROC map used and CH2 lunar map.

References

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