IDENTIFYING PLANETARY MATERIALS BY COMBINING A CUSTOM MINERALOGICAL DATABASE WITH MACHINE LEARNING BASED MULTI-SPECTRAL CLASSIFICATION.

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Introduction: The ESA-PANGAEA Mineralogical Toolkit is a set of analytical techniques aiming to enhance the recognition of planetary materials. It includes a custom publicly available database called the PANGAEA Mineralogical Database (MinDB), which contains information on all known minerals found on the Moon, Mars, and other planetary bodies [1]. This database then serves as the basis for a spectral classification system using machine learning (ML) to perform in-situ spectroscopic identification of minerals and their compositions [2]. Developed and tested together in the context of ESA's astronaut field science training using analogue environments, PANGAEA, the mineral library, and recognition software are conceived as real-time decision support tools for future planetary surface exploration missions.

PANGAEA Mineralogical Database: The MinDB [1] can be viewed as two distinct products: a catalogue of petrographic information (meta-data) and an analytical reference library. The catalogue consists of petrographic information on all currently known minerals identified on the Moon, Mars, and in meteorites. The catalogue is envisioned to provide essential analytical in-field information for rapid identification and understanding of significance during geological exploration. Each mineral entry includes: IMA recognized name, chemical formula, mineral group, surface abundance on planetary bodies, geological significance in context of planetary exploration, number of collected VNIR and Raman spectra, their spectral discoverability, and features. The database was compiled through systematic literature research, followed by the careful intercomparison of all mineral characteristic information. The second major part of the MinDB is a customized library of analytical data from all known planetary terrestrial analogue minerals. This covers reflective Visual-to-Near- & Shortwave-Infrared (VNIR), Raman vibrational (molecular) spectroscopy, Laser-Induced-Breakdown (LIBS), and X-Rays Fluorescence (XRF) atomic spectroscopy. This library also includes a set of reference spectra for evaluating the detectability of minerals with different analytical methods. The archive consists of high-quality spectra collected from available open access on-line catalogues, such as RRUFF (Raman), USGS, RELAB, ECOSTRESS (VNIR), and our own collection of spectroscopic measurements of planetary analogue minerals taken from different collections and synthetic spectral libraries, such as LIBS NIST, see [2].

Machine Learning (ML) software for recognition of minerals from multispectral data: To utilize the MinDB for *in-situ* real-time identification of minerals and their compositions from the output of analytical tools, we also developed methods that combine material characteristics, mineral structure (obtained with VNIR and Raman spectra) and chemical composition (from XRF and LIBS spectra) to achieve identification. To achieve this, we evaluated various ML approaches used to identify mineral species from single analytical methods (Raman, VNIR or LIBS), and developed a flexible and modular algorithm that can classify minerals either from one or pair-combined spectroscopic methods. Our new approach was then evaluated using our customized library of spectroscopic data from the MinDB. Our cross-validation tests show that multi-method spectroscopy paired with ML paves the way towards rapid and accurate characterization of minerals [2], as well as improving the quantification of mineral abundances in rocks and soils using ML-based spectral unmixing.

PANGAEA Mineralogical Toolkit as an Analytical Toolset for Planetary Surface Exploration: The PANGAEA Mineralogical Toolkit is envisioned as a part of the Electronic Fieldbook ToolSuite (EFB) [3], a deployable system supporting field science operations. The EFB can interface with handheld spectrometers intended for planetary exploration, simultaneously feeding their measurements into the embedded Mineralogical Toolkit. Combined with various spectral analytical tools linked to the EFB, the instrument agnostic nature of the Mineralogical Toolkit will enable fast and reliable in-situ recognition of rocks and minerals, thus becoming a crucial decision support tool for future human and robotic planetary surface exploration missions. The first field tests of the PANGAEA Mineralogical Toolkit combined with a portable spectrometer linked to the EFB during ESA's training and analogue testing programs, PANGAEA and PANGAEA-X by astronauts, planetary scientists, and operations engineers, have demonstrated the system's high prediction accuracy and operational efficiency.

References: [1] Drozdovskiy, I. et al. 2020, *Data in Brief*, 31, 105985. [2] Jahoda, P. et al. 2020, *The Analyst*, 146(1), pp.184-195. [3] Turchi L. et al. *Planetary Space Science*, 197, p.105164.