PHYSICS-INFORMED MACHINE LEARNING TO IDENTIFY FEATURES IN LCROSS NIR DATA. R. L. Fandozzi[1,2], A. D. Bravenec[4], J. W. Boyce[4], J. J. Gillis[2,3]. [1]McKelvey School of Engineering, Washington University in St. Louis, [2]McDonnell Center for the Space Sciences, Washington University in St. Louis, MO 63130, USA; [3]Department of Physics, Washington University in St. Louis, MO 63130, USA; [4]NASA Johnson Space Center, Houston, TX 77058; (f.raynah@wustl.edu).

Introduction: The main goal of the Lunar Crater Observation and Sensing Satellite (LCROSS) mission was to determine the presence and composition of ice in a permanently shadowed region (PSR). Near the lunar poles, permanently PSRs provide stable cold traps where temperatures are consistently below 120 K [1], allowing for the accumulation and long-term retention of volatile species, including water ice. LCROSS targeted one such PSR near the Moon's South Pole [2], the crater Cabeus (84.9°S 35.5°W), with average temperatures of about 37 K [1], making it a prime location to detect ice deposits.

The LCROSS mission executed a controlled impact experiment. It was comprised of two distinct impact events. The first, the spent ATLAS V upper-stage Centaur rocket from the co-manifested Lunar Reconnaissance Orbiter (LRO). Four minutes later, the LCROSS shepherding-spacecraft (S-S/C) struck the Moon; the velocity of both impacts was roughly 2.5 km/s. The S-S/C transmitted real-time observations from approximately four minutes before the Centaur's impact until nearly one second prior to the spacecraft's own collision. Descending through the Centaur's impact ejecta plume allowed visible and near-infrared (NIR) spectrometer and cameras to acquire data to characterize the plume's morphology, evolution, and composition. Colaprete et al. [2] applied a stepwise linear fitting approach to the LCROSS NIR spectra, modeling total absorbance as a linear combination of the manually selected species-specific spectral contributions, using a reduced chi-squared analysis to assess goodness-of-fit.

NIR Analysis with Machine Learning: Building on [2], we propose to reanalyze the LCROSS NIR data using an expansive and customized database of possible ices, salts, gasses, and minerals. Cutting edge machine learning techniques will be employed to identify and quantify species. Physics-informed machine learning offers the advantage of integrating data with mathematical physics, enabling robust analysis even in contexts with limited understanding and high-dimensionality [3].

We plan to implement a supervised, physics-informed machine learning framework that leverages multiple spectral features simultaneously, with the goal to potentially identify new species or offer new constraints on previously identified species within the hundreds of files of LCROSS NIR data.

Given that the spectral features of water ice vary systematically – depending on variables including the temperature, phase state (crystalline versus amorphous), and grain size – traditional diagnostics have relied on straightforward linear models or comparative fitting procedures to identify ice and even estimate ice temperature or phase [2, 4-6] (Fig. 1). However, the complete interplay among band center, width, and depth means that any single parameter model may fail to capture the full behavior of the system. Further, the system's complexity greatly increases when mixtures, rather than pure endmember components, are considered.

The goal of using physics-informed machine learning and a customized database is to provide new, quantitative constraints on species identified in LCROSS NIR spectra. Automation will allow analyses of the full NIR data set, which is critical for understanding the time-varying dependencies of ejecta plume composition.

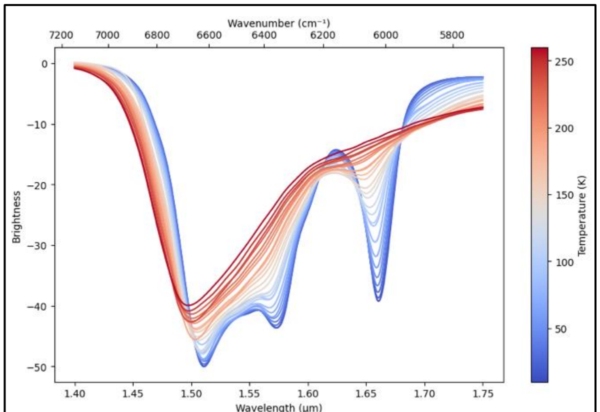

Figure 1: Illustration of the temperature dependence of H_2O ice, plotted using the data from [4]. The data points are sampled at 10 K intervals, spanning temperatures from 20 K to 270 K.

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