REFLECTANCE MODELING OF SPECTRA OF THE WELLS LUNAR GLASS SIMULANTS. K. R. Stockstill-Cahill¹, D. T. Blewett¹, J. T. S. Cahill¹, B. W. Denevi¹, S. J. Lawrence¹, and E. I. Coman¹,¹ Johns Hopkins University Applied Physics Laboratory, Laurel, MD 20723, USA, ³Arizona State University, Tempe, AZ 85287, ²Washington University, Dept. of Earth and Planetary Sciences, St. Louis, MO 63130, USA.

Introduction: Silicate glasses are an important constituent in the regolith of airless planetary bodies and knowledge of glass reflectance characteristics is important for remote-sensing studies of the Moon, Mercury, and asteroids. We recovered reflectance spectra for 20 vacuum-melted lunar glass simulants measured by Wells [1], which cover a wider range of Fe and Ti contents (0-17.5 wt.% FeO and 0-15 wt.% TiO₂) and a wider wavelength range than the better-known Bell et al. study [2]. We examine the spectra in terms of known absorptions, explore the relationship between UV spectral parameters and composition, and apply the Hapke radiative transfer model to predict the reflectance spectra of the Wells glasses. The imaginary part of the refractive index (k) at each wavelength was computed based on the Ti and Fe composition using the linear relationship presented by Wilcox et al. [3] and with a new linear-exponential hybrid relationship.

Method: We digitized the spectra presented in the figures of [1]. Spectra for seven of the samples were bidirectional reflectance plots. For the remaining samples, data were presented in terms of the bidirectional remission function \( W = (1-\alpha)/\alpha \), where \( \alpha \) is the single-scattering albedo. Therefore, it was necessary to convert from the \( W \)-function spectra to single-scattering albedo and then back to bidirectional reflectance using the early form of the Hapke bidirectional reflectance equation presented in [1]. In addition, most spectra were plotted in energy space (wavenumber on the x-axis). Spectra in energy space tend to have a higher density of points in the shorter-wavelength region (ultraviolet-visible) of the spectrum and a coarser sampling in the near-infrared. Therefore, after we converted from wavenumbers to wavelength (in \( \mu \)m), we resampled the reflectance spectra to a standard, evenly-spaced set of wavelengths. In Wells [1], spectra were presented for all 20 glasses in a <37 \( \mu \)m grain size split and for five glasses in a 37-74 \( \mu \)m grain size split.

In this study we applied the radiative transfer model of Hapke [4, 5] to predict the bidirectional reflectance spectra of the glasses based on their Ti and Fe compositions in a forward modeling approach [6, 3]. First, the Fe and Ti abundances of a given glass were input into either a linear model [3] or a hybrid linear-exponential model (which employs an exponential fit from 0.35-0.77 \( \mu \)m and the standard linear fit from 0.2-0.34 \( \mu \)m and 0.78-2.5 \( \mu \)m) to calculate the appropriate optical constants for that glass. These optical constants were then input into the Hapke radiative transfer model as implemented by [6] to derive a modeled bidirectional reflectance spectrum. Model parameters include average grain size, incidence angle (30º), emergence angle (30º), and phase angle (60º). Average grain size of each grain size split was determined iteratively and determined to be 23 \( \mu \)m for the <37 \( \mu \)m particle size split and 65 \( \mu \)m for spectra of the 37-74 \( \mu \)m particle size split.

Results: The success of either linear or hybrid modeling for <37 \( \mu \)m particle size split depends strongly upon the abundance of FeO and, to a lesser extent, on the abundance of TiO₂. In general, glasses that contain abundant TiO₂ but no FeO (e.g., glass 33) are not well modeled; conversely glasses with abundant FeO but no TiO₂ (e.g., glass 14) can be well modeled (Figs. 4 and 6). This may reflect the ability of the models to fit absorptions near 1 and 2 \( \mu \)m that result from Fe²⁺ in a distorted octahedral site similar to the M2 site in pyroxenes [7]. However, the linear and hybrid models have significant differences in their abilities to model spectra of glasses across a wide compositional range.

Linear model. Figure 1 displays the model results for five compositionally-representative linear models in order of increasing FeO + TiO₂ content. Comparison of the model spectra with the measured spectra reveals that the samples rich in Fe and Ti are best modeled by the linear relationship. Indeed, the glasses with very low FeO and/or TiO₂ (e.g., glasses 10 and 33) are very poorly modeled using a linear relationship between the composition and the optical constants (Figure 1). This is probably because the linear model was developed using the Fe- and/or Ti-rich glasses of [2].

Hybrid model. Figure 2 displays the model results for five compositionally representative hybrid models in order of increasing FeO + TiO₂ content. For Fe- and Ti-poor glasses, the hybrid model provides a better fit to the measured spectra (compare Figures 1 and 2), because this model for \( k \) is based on the wider compositional range of the Wells glasses. Careful inspection of the model spectra for both models reveals that the hybrid models do not improve fits for glasses with abundant FeO and TiO₂ when compared to the linear model results. Specifically, there is a poor fit in the wavelength range (i.e., 0.35-0.77 \( \mu \)m) that is modeled using an exponential fit for the optical constants [8].
Future work: Moving forward, a first step would be to develop a new linear model based on a larger compositional range. Ideally, the linear relationship between composition (FeO + TiO$_2$) and the $k$ coefficient from [3] would be recalculated including both Bell and Wells glass spectra as well as spectra of glasses similar to the Apollo red, orange, yellow and green glasses. These glasses would need to be synthesized and their compositions and spectral reflectance measured to be included in the model. This would allow the spectral modeling of glasses to be extended to low Ti, low-Fe planetary surfaces, such as Mercury, as well as the high-Fe, high-Ti surface of the Moon. A linear model based on a wider compositional range may prove to be a better method to model the FeO and TiO$_2$ composition of glasses on planetary surfaces.

In addition, the modified Gaussian model (MGM) previously used to model mineral abundances in pyroxene mixtures [9] may prove to be a useful tool in refining spectral modeling of lunar glasses. MGM modeling can be used to deconvolve spectra of mixtures into absorption bands that correspond to absorptions identified in mineral endmember spectra because the relative band strength varies logarithmically with modal abundance [9]. Preliminary work on MGM modeling of the $k$-spectra of synthetic lunar pyroclastic glasses ranging from ~0.5-15 wt.% TiO$_2$ with nearly constant FeO abundance (~20 wt.%) was reported by [10]. That study successfully fit the $k$-spectrum using the gaussian fit in the UV-NIR and band centers were well predicted, but had problems predicting the relationship between FeO and absorption strengths [10]. Although the MGM modeling method of glasses holds promise, a wider range of glass compositions is necessary to better understand the location and shape of UV-Vis absorptions as they relate to FeO and TiO$_2$ [10].