**The Effect of Grain Size and Abundance on the Deconvolution of Mixtures Using the Shkuratov Model.** A.A. Martone[1] and T.D. Glotch[1], [1] Stony Brook University (255 Earth and Space Sciences, Stony Brook University, Stony Brook, NY 11794-2100 )

**Introduction:** In this work we use the Shkuratov radiative transfer model to obtain mineral optical constants, and test the model's ability to deconvolve reflectance spectra of mineral mixtures and determine mineral grain sizes and abundances. The tests of the model focus on the effects of grain size and end member concentrations on the accuracy of the model.

The Shkuratov model approximates scattering through parallel plates, eliminating a dependence on incidence angle. It relies on a priori estimates of the real index of refraction (n), volume fraction filled by particles (q), and optical path length, or particle size (S), to determine the imaginary index of refraction (k) from reflectance spectra [1]. Values of k derived from this model are dependent on S, even though the value is an intrinsic mineral property and should be the same for a mineral at all grain sizes (figure 1). Poulet and Erard [2] discuss this and found that k values are substantially more accurate when calculated from mineral spectra of several sizes. In this study, we report the effect of singular particle size k values on the results of the deconvolution of mixtures.

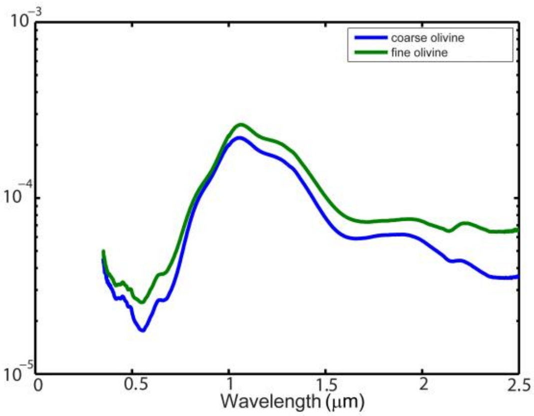


**Figure 1:** comparison of k values for the coarse (125-250μm) and fine (63-90μm) olivine

Our Matlab deconvolution code uses an optimization function that finds the minimum for a nonlinear multivariable function within set constraints. We employ the MultiStart algorithm which allows us to run the optimization from multiple points to increase the certainty that a global minimum has been found; it becomes increasingly difficult to find a global minimum when there is a large number of unknowns (ie: for a mixture with many end members).

**Two Component Mixtures:** We use two and three component mixtures consisting of olivine (OLV; 2 size fractions), labradorite (PLG), augite (CPX), and enstatite (OPX). The potential accuracy of the model is demonstrated with the OPX/CPX mixture (2:1 mass fraction ratio). The abundances were determined with errors of 3% and 6%, respectively, with reasonable grain sizes (both have particle size ranges from 90-125μm). The fit of the spectrum is shown in figure 2. OPX and CPX are kept in this 2:1 ratio for the 3 component mixtures.

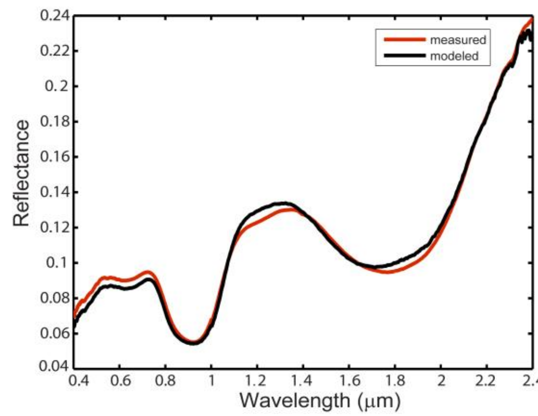


**Figure 2:** measured and modeled spectrum of OPX/CPX mixture

CPX and OLV were mixed using fine (63-90μm) and coarse (125-250μm) size fraction of OLV in 1:2, 1:1:, and 2:1 mass ratios. The mixtures with coarse olivine provided more accurate model results for all three ratios compared to the finer olivine; the finer olivine mixture had a errors of 57% and 61% for the 1:1 mixture, 27% and 53% for the 2:1 mixture, and 29% and 15% for the 1:2 ratio, while the coarser olivine mixtures had errors of 22% and 22% for the 1:1 mixture, 15% and 36% for the 2:1 mixture, and 44% and 23% for the 1:2 mixture. All these results also produced particle sizes with reasonable agreement to the actual sizes. Mixtures in a 1:2 ratio were also made using a coarser CPX size fraction with a particle size range of 180-250 μm. For the coarser olivine mixture this produced errors of 14% and 8% (with a modeled CPX grain size of 500 μm), and the fine olivine 76% and 40%.

The effect of the size-dependent k value was observed by using the fine olivine k for the mixtures with coarse olivine, and vice versa. These effects are unpredictable, in some instances improving accuracy and in others decreasing it. The effect, however, is small; the difference is ≤ 2% for 14 of the 16 mixtures, the other two have a 5% and 7% difference.

Mixtures of CPX and PLG (125-250 μm) were made in 1:1, 1:2, and 2:1 ratios. These consistently overestimated the PLG by 15-20%, while the CPX errors ranged from 21%-45% with the 2:1 mixture producing the smallest error and the 1:2 mixture producing the largest. The grain sizes were within reason for all mixtures except the 2:1 ratio which produced a CPX size about three times larger than the actual size.

**Three Component Mixtures:** The three component mixtures consisted of OPX and CPX (kept in a 2:1 ratio), and either coarse OLV or PLG as an additional end member. Three mixtures were made for each in a (CPX+OPX):end member ratio of 1:1, 1:2, and 2:1. For the PLG-bearing mixtures, labradorite abundance was overestimated by the same percentage as it was in the two component mixture, OPX was always underestimated, and CPX was always overestimated. The PLG and OPX grain sizes were reasonable, but the CPX grain size was considerably larger than the actual size fraction. Despite these errors, a fitted spectrum is produced with a RMS value of .0947% (Figure 3). For the OLV-bearing mixtures, the OPX was again underestimated for all three ratios, CPX was overestimated for the 1:1 and 2:1 ratios and underestimated in the 1:2 ratio, olivine was overestimated for the 1:2 and 2:1 ratios and underestimated for the 1:1 ratio. As with the labradorite end member mixtures, the CPX grain size was drastically larger than the actual size fraction.

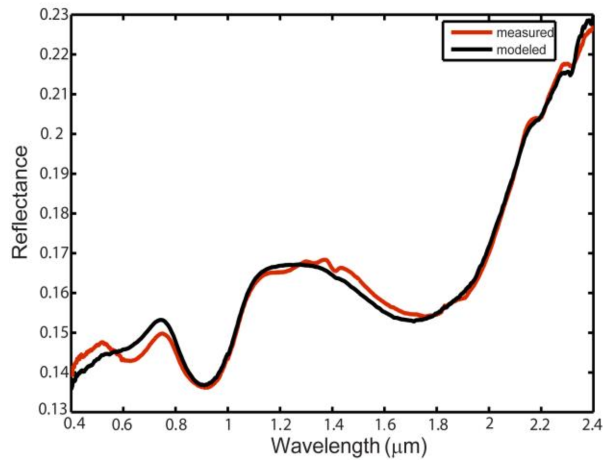


**Figure 3:** OPX+CPX/PLG measured and modeled spectrum

**Discussion and Conclusions:** The frequent modeling of a larger than actual grain size for CPX is likely due to the fact that CPX band contrast in the VNIR spectral range is poorly correlated with grain size [2]. The similarities between the CPX and OPX bands may make it difficult to distinguish between the two when another end member is introduced to the mixture. The OLV-bearing two component mixtures were modeled more accurately when the coarse OLV was an end member. In future work we will expand these tests by incorporating a different CPX end member and using additional size fractions of each end member.

**References:** [1] Yurij Shkuratov et al. (1999) *Icarus 137, 235-236* [2] F. Poulet and S. Erard (2004) *JGR, Vol.109* [3] L. Moroz and G. Arnold (1999) *JGR, Vol. 104*

**Table 1:** percent errors of abundances for mixtures

| | 1:1 | 1:2 | 2:1 |
|---|---|---|---|
| OPX:CPX | - | - | 3%/6% |
| CPX:OLV(c) | 22%/22% | 23%/44% | 36%/18% |
| CPX(c):OLV(c) | - | 14%/18% | - |
| CPX:OLV(f) | 61%/57% | 15%/29% | 53%/27% |
| CPX(c):OLV(f) | - | 76%/40% | - |
| CPX:PLG | 33%/40% | 45%/27% | 21%/52% |
| (OPX+CPX):PLG | 38%/36%/22% | 52%/5%/19% | 65%/260%/13% |
| (OPX+CPX):OLV | 54%/160%/8% | 39%/71%/27% | 61%/32%/66% |