Purpose: To investigate the feasibility of accurate quantification of concentrations of mixtures of K-edge contrast agents in spectral Computed Tomography (CT) imaging based on a novel maximum likelihood based method.

Methods: Calcium, gold, and iodine solutions of various concentrations were prepared in vials and placed in phantoms for imaging at 100 kVp with a Cadmium-Zinc-Telluride (CZT) photon counting detector. The linear attenuation maps were reconstructed in 5 energy bins, whose boundaries were 22, 34, 60, 80, and 100 keV. A novel maximum likelihood-based algorithm for material decomposition was developed. Summing over the energy bins, on a pixel-by-pixel basis, this procedure takes into account the reconstructed linear attenuation coefficient, its associated noise, and the tabulated mass attenuation coefficient of each material of interest, to determine a cost function. The unknown parameters to be fitted by optimization by the MINUIT optimizer (from CERN) of the cost function are the concentrations of the materials of interest at each pixel. The result is a density map image for upper limits on the concentration of each material.

Results: Multiple material decomposition of the spectral CT phantoms according to this method yields reliable estimates of concentrations. The upper limits on concentrations are linearly correlated with known concentrations.

Conclusions: This study indicates that the problem of decomposition of multiple materials of interest may be facilitated by optimization in the image domain, based on linear attenuation values, and using log-likelihood and upper limit techniques. This technique can be used for analysis of the spectral CT data.