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Carolyn K. Cuff* (ccuff@westminster.edu), Box 13, Westminster College, New Wilmington, PA 16172-0001. *Getting inside the black box of chemometrics: interdisciplinary research between statistics and chemistry.*

Chemometrics can be defined as analyzing measurements made on a chemical system or process via application of mathematical or statistical methods. Many such analyses are often done by chemists via a “black box approach.” Chemists, then, often cannot explain the statistical process behind the analysis. With a good introductory statistics foundation, we believe students are capable of learning and explaining what is happening in the black box. Our chemometric work, a collaboration between math and chemistry students and professors, has focused on calibration curves. In undergraduate chemistry work, univariate calibration curves are typically used. They allow for the determination of concentrations of a single component (compound, element). Interactions between two components are harder to model, and the calibration curves are not as accurate as when there is no interaction. Principal component analysis can be used to create more accurate calibration curves and, therefore, better predictions of the concentrations. Our goal is to have students create the statistical analysis of the black box to determine the concentration of two heavy metals in frack water waste. This paper examines the successes (and frustrations) of the interdisciplinary work. (Received September 08, 2014)