Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) of Biomass and Coal: A Chemometrics Analysis

Guilin Jiang,¹ Bonnie J. Tyler,³ Larry Baxter,² Matthew R. Linford¹

1. Department of Chemistry and Biochemistry, 2. Department of Chemical Engineering, Brigham Young University, Provo, UT 3. Department of Chemical Engineering, University of Utah, Salt Lake City, UT

Objectives

Perform Principal Components Analysis (PCA) and Cluster Analysis (HCA) of multivariate ToF-SIMS data of biomass and coal samples to explore the inter-sample and inter-variable relationships.

<u>PCA</u>: find the principal components (eigenvectors and values) among a set of data based on variation: Advantages of PCA $\sum_{i=1}^{3} x_{i}^{2}$

•Quantitative analysis •Reduce size of huge data sets •Keep important information •Remove user bias •Efficiently use the data

<u>Cluster Analysis</u>: find the similarity among a set of data based on Euclidean distance:



80 peaks (variables) were chosen from each positive ToF-SIMS spectrum (17 coal samples and 6 biomass samples) forming a 23 x 80 data matrix. The data matrix was then row scaled and standardized (mean centered and divided by its standard deviation).



•) –	PC	Var.	lot. Var.	PC	Var.	l ot. Var.	
>/	1	54.40	54.40	7	1.32	95.64	
	2	23.17	77.58	8	1.05	96.70	
	3	7.10	84.68	9	1.01	97.71	
	4	6.16	90.84	10	0.68	98.39	
	5	2.02	92.86	11	0.45	98.84	
	6	1.46	94.32	12	0.33	99.17	

Fig. 1. Variations captured by principal components



Fig. 2. PC1 separates biomass from coal (up), and PC2 separates coal and biomass individually.



Fig. 3. PC3 and PC4 (right) separate biomass (and coal) individually, but not from each other.



Fig. 4. Similarity separates biomass from coal.

Conclusions:

- Multivariate analyses show that the spectra of coal and biomass are distinctly different.
- More chemical information is extracted from the data by standardization than by row scaling alone.
- Principal Components Analysis and Cluster Analysis help build the case for ToF-SIMS as a useful tool for fuel analysis.

Future work:

 Do PLS (partial least squares) on the data to predict coal properties from ToF-SIMS data.