A Chemometrics Analysis of ToF-SIMS Data of Coal

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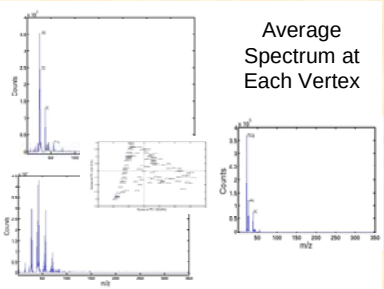
Sample Preparation and Analysis

- Coal samples were ground with a mortar and pestle
- They were immediately mounted on double sticky tape
- 500μm x 500μm regions were then analyzed by ToF-SIMS

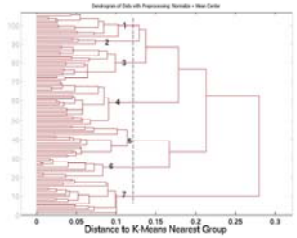
Why do chemometrics/ bioinformatics?

- Find outliers, and find them quickly.
- Understand the chemical basis of variation between samples, or between samples and outliers.
- Quickly categorize and/or see relationships between samples.
- Build regression models.
- Variable reduction.
- Avoid peak choice bias and user bias.
- How else can you deal with a dozen or more spectra that have thousands of peaks in them without ignoring a significant fraction of the information that is them?

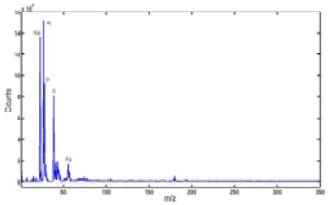


Average Spectrum at Each Vertex

Dendrogram from a Cluster Analysis

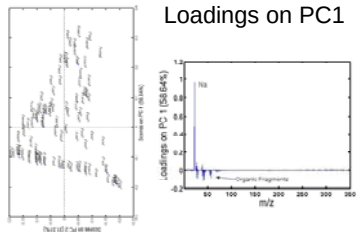


Average ToF-SIMS Spectrum of Coal Samples



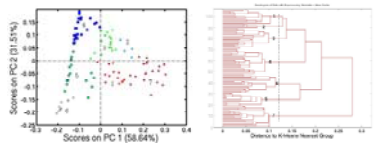
Chemometrics Analysis Methods

- Principal Components Analysis (PCA)
- Cluster Analysis
- Multiple Linear Regression (MLR)
- …

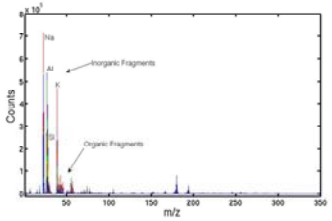


Loadings on PC1

Integrating the PCA and Cluster Analyses: Seven Clusters

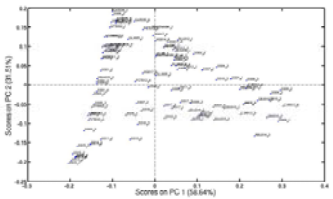


All of the ToF-SIMS Spectra Superimposed

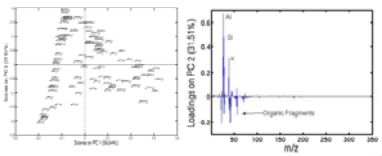


Scores Plot of PC1 vs. PC2

(PC1 and PC2 account for just over 90% of the variance in the data.)



Loadings on PC2



R^2 Values for Regression

Properties	R^2 after mean centering	R^2 (95 var.) log scaling	R^2 (85 var.) log scaling	R^2 (75 var.) log scaling
MOISTURE	0.973	0.995	0.991	0.979
VOLATILE MATTER	0.561	0.996	0.989	0.966
ASH	0.774	0.990	0.936	0.912
CARBON	0.078	0.997	0.947	0.906
HYDROGEN	0.133	0.992	0.963	0.943
NITROGEN	0.540	0.998	0.986	0.980
SULFUR	0.820	0.986	0.960	0.929
HEATING VALUE	0.104	0.997	0.960	0.934
CHLORINE	0.990	0.997	0.972	0.939
OXYGEN	0.892	0.999	0.993	0.979
H:C	0.905	0.999	0.993	0.979
O:C	0.158	0.992	0.974	0.931
SIO2	0.540	0.994	0.986	0.965
AL2O3	0.597	0.994	0.989	0.963
TIO2	0.549	0.974	0.961	0.928
FE2O3	0.754	0.965	0.937	0.873
CAO	0.985	1.000	0.998	0.988
MGO	0.960	0.999	0.993	0.978
NA2O	0.959	0.998	0.993	0.984
K2O	0.832	0.997	0.985	0.969
P2O5	0.907	0.999	0.974	0.914