The main objective of this project was to develop a sulfur prediction model using Python that utilizes the ultrahigh resolving power of FT-ICR (Fourier Transform-Ion Cyclotron Resonance) mass spectral data to deconvolve data collected from the lower resolving power Time-of-Flight mass spectrometer (TOF-MS). The ultrahigh resolving power of the ICR mass spectrometer facilitates the resolution and separation of the 3.4 mDa split, which represents mass difference between isobaric compounds that differ in mass by C₂ vs. SH₄. This split is critical for the identification of sulfur in petroleum crude oils and provides an insight into its complex structure, which is necessary for the development of effective upgrading and refinery strategies routinely applied in oil production.

**DATA PROCESSING**

**Basic Algorithm in Python**

1. Import data file from PetroOrg
2. Sort data
3. Find the centroid using a polynomial fit equation
4. Separate out 3.4 mDa mass splits
5. Plot 3.4 mDa mass splits

**Challenges**

- Strategizing how to look for 3.4 mDa mass splits
- Requiring increased precision to calculate error using ppm
- Determining a percent error to identify sulfur mass split

**Visualization of Original negative ESI FT-ICR-MS data:**

**Visualization 3.4 mDa splits:**

**SAMPLE PREPARATION**

The sulfur prediction model was implemented using Python. The program reads in a data file from PetroOrg, sorts the data, calculates the centroid using a polynomial fit, then identifies 3.4 mDa mass splits before producing a visualization of the processed data. This research is ongoing and visualization of the 3.4 mDa mass splits was the initial task prior to using the software to deconstruct TOF-MS data. This work will help identify sulfur using low-resolution TOF-MS, producing valuable information regarding sulfur speciation and chemical composition for oil companies. As a result, more oil could be used as fuel rather than to pave roads as asphalt or one of the many alternative uses of crude oil with sulfur.

**CONCLUSION**

The oil samples containing the heteroatom sulfur were ionized into the gas phase using negative electro spray ionization (ESI). Sample preparation involved using a 1:1 ratio of toluene and methanol with 0.0125% TMAH by volume. The samples were then analyzed with a custom built FT-ICR mass spectrometer equipped with a 9.4 T superconducting magnet [5].

**REFERENCES**

7. http://commonwealthmagazine.org/transportation

**ACKNOWLEDGEMENTS**

This work was sponsored by the National Science Foundation Division of Materials Research through DMR-11-57490, the Florida State University Future Fuels Institute, and the State of Florida.