Fourier Transform Ion Cyclotron Resonance Mass Spectrometry – the analytical tool for heavy oil and bitumen characterization

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Petroleum geochemistry has been driven by analytical advances since the development of gas chromatography in the 1950's and practical computerized GCMS technologies in the 1970's heralding, in the 70's and 80's, the development of practical biomarker technologies and most of the source rock facies and maturity molecular concepts that we still use today. Another chapter in the development of petroleum geochemistry came with the development of kinetic models of petroleum generation and sophisticated basin modeling tools in the 1980's and 90's. What awaits us in the 21st century? In the 1970's another analytical development was also taking place, namely that of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICRMS) by Marshall and Comisarow at the University of British Columbia. Nearly 4 decades later FTICRMS has evolved into a commercially available front line tool capable of analyzing several hundred thousand components in a petroleum mixture at once. It is likely this analytical technology will usher in an equally dramatic revolution in geochemical capability, comparable to or greater than the molecular revolution that grew from GCMS technologies being cheaply available. Already Marshall and Rodgers at the High Field Magnetic Lab in Florida have coined the term "Petroleomics" to reflect the molecular resolution and information content available in FTICRMS analysis of petroleum comparable to the information in the human genome. So from the perspective of a practicing petroleum geoscientist what are the challenges and opportunities the FTICRMS revolution brings?

Currently, just as in the early days of routine GCMS, instruments have "personality" and component quantitation and very variable component ionization efficiency is a major issue but these problems will likely be quickly resolved. Data sets are measured in the gigabytes and geochemists are learning the tricks of the bioinformaticians and others. Data processing is perhaps one key to the revolution that is unfolding. Current GCMS based petroleum geochemical protocols quantitatively determine perhaps a few hundred components. FTICRMS potentially can resolve 1000 times this number of components, which when quantitated and with accompanying molecular formulae, opens the door, *in principle,* to computational routes to fluid property and phase behavior calculations directly from molecular analysis. Interaction of genes, not the genome itself describe biology and so with petroleum, interaction of the multitude of hydrocarbon and non-hydrocarbon components, not the components themselves control fluid and other properties and it will be definition of this "interactome" that will be key to unlocking the potential of petroleomics.

Geochemical assessment of severely degraded oils is currently not easily achieved as the most common markers are often destroyed by the degradation process. We describe applications of FTICRMS and data processing to study heavy oil and oil sands bitumen variability, identify some novel biomarkers of potential paleoecological significance and we discuss routes to defining the petroleum "interactome".