FTICR-MS – towards reaction systems models in petroleum geochemistry

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Over the last five decades, Petroleum Geochemists have developed a great selection of tools and molecular markers, or proxies, to better understand the processes involved in the generation, migration and alteration of petroleum. Unfortunately, several of these proxies are altered during in situ biodegradation in oil reservoirs and are thus, not available for petroleum system studies in many biodegraded oil provinces. Historically, most of the petroleum system proxies used by geochemists are predominantly hydrocarbon in nature, but recent advances in analytical technology, FTICR-MS, now permit routine analysis of tens of thousands of molecules containing polar functional groups as they occur in oil which are commonly not accessible using standard GC-MS technology. These non-hydrocarbon species, in addition to providing new and more robust petroleum system proxies, are also the most critical components, to assess in terms of understanding fluid rock interactions and key phenomena such as solid phase wettability, emulsion formation, water washing effects, and petroleum migration to name but a few topical areas. These fluid-solid and fluid-fluid interactions mediated by petroleum non-hydrocarbons can be termed interfacial phenomena and are a badly neglected area for petroleum geochemists. FTICR-MS is still in its early days and needs further developments especially to improve its rudimentary quantitation capabilities but it is already starting to produce interesting and usable results with practical implications for organic and petroleum geochemists.

In this presentation, we would like to give an overview of recent advances in improving the quantitation capabilities of FTICR-MS and how to convert the tremendous amount of produced data now available into useful information for applications in the areas of petroleum geochemistry. Recent software developments, a better understanding of the competition of oil constituents for ionization resulting in different response factors and the use of statistical methods such as chemometrics allows us to develop reaction systems models for several new petroleum system proxies.