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PETROLEOMICS

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1 What is the meaning of "petroleomics"?

Prof. O. Mallinz (Schlumberger, 2007) introduced the concept of petroleomike as a new scientific direction in the study of petroleum systems, which by analogy with genomics in biology, is based on the concept of the development in each oil distribution system unique continuous series of different size and solubility of resin-asphaltene components in the hydrocarbon matrix.

Petroleomics is a new field in petroleum chemistry engineering I am launching through my publication. "To understand function, study structure," said Francis Crick, Nobel Prize winner for revealing the chemical structure of DNA, a discovery that led to genomics. We envision petroleomics being to petroleum science what genomics is to medical science. In short, medicine traditionally treats patients based on symptoms, and the vision of genomics is to predict and treat medical concerns even before symptoms appear. Petroleum science has, similarly, been phenomenological. Establishing structure-function relationships has been precluded in petroleum science because nobody knew the petroleum chemical structure.

This is all about to change. Petroleomics promises the ability to predict petroleum properties based on the foundation of elucidating the chemistry of all constituents in a crude oil. In addition, it is necessary to get information concerning Downhole Fluid Analysis in order to exploit petroleum chemistry to understand reservoir architecture.

2 What constitutes a petroleome?

The petroleome is the complete listing of all chemical constituents in a crude oil, the "genome" you might say of a crude oil. There has been no debate about the significance of understanding light end chemistry. Does the oil have H2S, CO2? These are chemically specific questions of great concern. However, for heavy ends, there has been no consensus as to what the chemistry is.

The chemistry of the heavy ends is now largely resolved, a major accomplishment. Furthermore, we show the evolution of the petroleome — which consists of ~ 40,000 chemical constituents. Achieving the petroleome is now feasible with the advent of the ultra-high-resolution mass spectroscopy invented by Professor Alan Marshall, also utilizing Electro-Spray ionization (ESI), invented by John Fenn, which won the Nobel Prize in 2002.

3 Is there a "Global Petroleome Project"

Excellent question. At this stage, there are many players on the sidelines. When scientists first launched petroleomics, many scoffed at the idea. Heavy end analysis had been considered intractable. Their laboratory experiment has shown that heavy ends are not as complicated as first thought. These results are being confirmed in laboratories around the world and are documented. Now, petroleomics is being taken much more seriously.

Nevertheless, there is one more major development needed. By far the biggest problems in the upstream oil business have to do with the reservoir. What is the reservoir

architecture? What will be produced by sweeping extended transition zones in giant fields? But the petroleum chemistry community has been focused on flow assurance — admittedly a significant problem, but one which pales in comparison to reservoir issues. They are linking state-of-the-art chemical developments with the reservoir through Downhole Fluid Analysis (DFA). Once they show the application of advanced chemistry to reservoir concerns, operating companies will adapt in reasonable time. For example, a senior reservoir engineer with a major operator recently stated that use of DFA for reservoir fluid mapping should be as common as gamma ray logging for stratigraphy (which is done in every well). When advances in science and technology contribute to solving the industry's biggest problems, acceptance is rapid.

Petroleomics and Structure-Function Relations of Crude Oils and Asphaltenes.- Asphaltene Molecular Size and Weight by Time-Resolved Fluorescence Depolarization.- Petroleomics: Advanced Characterization of Petroleum Derived Materials by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS).- Molecular Orbital Calculations and Optical Transitions of PAH's and Asphaltenes.- Carbon Raman X-Ray Spectroscopy of PAH's and Asphaltenes.- Sulfur and Nitrogen Chemical Moieties in Carbonaceous Materials.- Micellization.- Insights into Molecular and Aggregate Structures of Asphaltenes Using HRTEM.- Ultrasonic Spectroscopy on Asphaltene Aggregation.- Asphaltene Self-Association and Precipitation in Solvents - AC Conductivity Measurements.- Molecular Composition and Dynamics from NMR Diffusion Measurements.- Application of the PC-SAFT Equation of State to Asphaltene Phase Behavior.- Application of Isothermal Titration Calorimetry in the Investigation of Asphaltene Association.- Petroleomics and Characterization of Asphaltene Aggregates Using Small Angle Scattering.- Self-Assembly of Asphaltene Micelles: Synchrotron, Simulation and Chemical Modeling Techniques Applied to Problems in the Structure and Reactivity of Asphaltenes.- Solubility of the Least-Soluble Asphaltenes.- Dynamic Light Scattering Monitoring of Asphaltene Aggregation in Crude Oils and Hydrocarbon Solutions.- Near Infrared Spectroscopy to Study Asphaltene Aggregation in Solvents.- Phase Behavior of Heavy Oils.- Selective Solvent Deasphalting for Heavy Oil Emulsion Treatment.- The Role of Asphaltenes in Stabilizing Water-in-Crude Oil Emulsions.- Live Oil Sample Acquisition and Downhole Fluid Analysis.- Precipitation and Deposition of Asphaltenes in Production Systems: A Flow Assurance Overview.

4 Conclusion

Petroleomics is a vision whose time has come. The foundations of asphaltene molecular structure are established; the hierarchy of petroleum colloidal structure is being revealed. Petroleum chemistry engineering specialists are now emboldened to address enormous problems, in particular via DFA. Petroleum science is now ready to join the pantheon of other scientific disciplines which abide by Francis Crick's axiom, "to understand function, study structure."

The oil and gas industry has a reputation — in my view undeserved — for being slow and conservative. In fact, the oil and gas industry rapidly tests and utilizes new technology. Nevertheless, to exploit optimally the latest developments, we need a partnership of visionaries in both operating and service companies to focus on overall production objectives. Scientists cannot be impeded by archaic adversarial relationships. In this way, they all benefit from new science and technology.

Development and using of power devices would have a really deep processing of oil, and hence the efficient use of valuable natural resources, without which it’s hard to imagine our modern life.