



geoconvention

Calgary • Canada • May 13-17 2019

Advances in Petroleomics approaches for petroleum systems assessment using ultrahigh resolution mass spectrometry – FTICR-MS

Thomas B.P. Oldenburg¹, Melisa Brown¹, S. Hossein Hosseini¹, Ygor dos Santos Rocha², Reinhard F. Sachsenhofer³, Steve R. Larter¹

¹University of Calgary, ²Petrobras (CENPES), ³Montanuniversität Leoben

Summary

Molecular petroleum geochemistry developments over the last five decades were mainly focused on saturated and aromatic hydrocarbons as those species were most abundant in crude oil and the available analytical technology (GC-MS) had vast limits for non-hydrocarbons (nitrogen, sulfur and oxygen (NSO) containing organic compounds). In recent years, with the advances in ultrahigh resolution mass spectrometry several applications for the assessment of petroleum systems were developed (e.g. Oldenburg et al., 2014 and 2017). The non-hydrocarbon fraction of crude oils and source rock extracts can make up a significant portion of petroleum, especially in heavy and extra-heavy crude oils. Due to its greater range in physicochemical properties compared to hydrocarbons the non-hydrocarbons have a high potential for the definition and understanding of geochemical properties and processes such as organic facies and maturity assessment, expulsion and migration distances, and alteration processes like biodegradation, water washing and solid bitumen generation.

Theory / Method / Workflow

In this study, we will review the current knowledge in petroleomics geochemistry and expand the range of reaction systems assessments of various processes occurring in petroleum systems. Using our 12T Bruker Solarix Fourier Transform Ion Cyclotron Resonance mass spectrometer (FTICR-MS) in three ionization modes (APPI-P, ESI-N, ESI-P) we investigated geochemical processes within several petroleum systems.

Results, Observations, Conclusions

Apart of several petroleum systems from the North Sea, Western Canadian Sedimentary Basin and Chinese basins, a comprehensive sample set was selected from the Alpine Foreland Basin (Molasse Basin) and Vienna Basin (Figure 1) which comprises several oils, source rocks and reservoir solid bitumen covering a broad range of geochemical processes affecting the composition of hydrocarbons and non-hydrocarbons such as facies variations, maturity, expulsion, lateral migration, TSR, biodegradation and solidification.

The results of sample sets from several petroleum systems will be discussed.

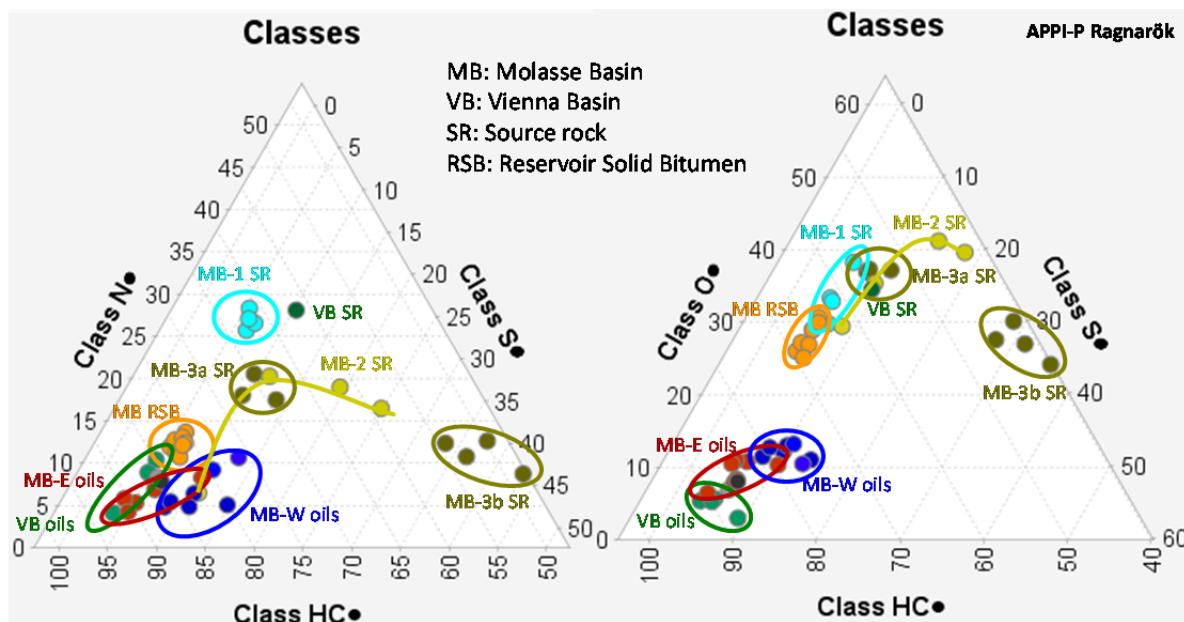


Figure 1 Triangular plots showing the variation of the relative distribution of hydrocarbons (HC) and non-hydrocarbons (N1, S1, O1) of oils, source rock extracts and solid bitumen from the Molasse and Vienna Basins.

Novel/Additive Information

Petroleomics is a novel molecular assessment tool for Petroleum Exploration and Production challenges.

Acknowledgements

We thank the FTICR-MS project consortium at PRG (Ecopetrol, Petrobras and Shell International) and the TESLA Phase II sponsor Petrobras for their financial support. Aphorist Inc. is thanked for providing access to the FTICR-MS data analysis and visualization software CaPA and Ragnarök. Bruker are thanked for their continued support, in the development of the University of Calgary FTICR-MS facility. In addition, we would like to thank NSERC (Canada), the Canadian Foundation for Innovation (CFI) and the Canada Research Chairs for research funding.

References

- Oldenburg, T.B.P., Brown, M., Bennett, B., Larter, S.R., 2014. The impact of thermal maturity level on the composition of crude oils, assessed using ultra-high resolution mass spectrometry. *Organic Geochemistry*, 75, 151-168.
- Oldenburg, T.B.P., Jones, M., Huang, H., Bennett, B., Shafiee, N.S., Head, I., Larter, S.R., 2017. The controls on the composition of biodegraded oils in the deep subsurface- Part 4. Degradation and production of high molecular weight aromatic and polar species during in-reservoir biodegradation. *Organic Geochemistry* 114, 57-80.