UNRAVELLING THE ROLE OF LITHOFACIES IN CONTROLLING ORGANIC MATTER COMPOSITION IN UNCONVENTIONAL SYSTEMS USING FT-ICR-MS

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Evolution of organic matter in sedimentary basins over geological times includes formation of kerogen, production of hydrocarbons, expulsion, migration, accumulation and possible transformation within the reservoir. Inorganic components, e.g. mineralogical composition, could play an important role in this evolution of organic matter (Murgich and Jesús Rodríguez, 1998). Jones et al. (1994) emphasized similarities in petroleum generation for shale and carbonate source rocks but stressed possible differences in migration. Carbonate source rocks tend to be more brittle, heterogeneous and tighter than clay rich source rocks, which makes them more prone to fracture and emit hydrocarbons more effectively. As defined by Jarvie (2012), unconventional resource systems include not only organic rich rocks which can generate and store petroleum itself but also juxtaposed organic lean intervals where generated petroleum can migrate into. Those juxtaposed organic lean units also may have different lithofacies than the organic rich units. Improved oil quality could be found in juxtaposed organic lean units, because short distance secondary migration leaves more heavy and polar compounds in the source.

To elucidate the controls that different lithofacies may have on the composition of organic matter in unconventional systems, we investigated samples from three different locations including carbonate-rich Niobrara Formation, biogenic quartz-rich Barnett Shale and clay-rich Posidonia Shale. All samples are of similar kerogen type (type II) and thermal maturity (0.88-1.02% Rc). Besides, they all have experienced intensive hydrocarbon generation and expulsion. For Niobrara Formation and Barnett Shale, samples were chosen from both, organic rich units and juxtaposed more carbonate or quartz rich units. Thus, lithofacies effects on organic matter within and between different unconventional systems are evaluated using (+)-APPI FT-ICR-MS with focus on retention and migration processes.

Differences in compound class distribution between those three sample sets can be observed. Posidonia and Barnett Shale have higher $(O_xN_y+N_y+O_x)$/hydrocarbons, N_2/N_1 and N_2O_1/N_1O_1 ratios. More polar compounds and compounds containing two nitrogen atoms are retained by Posidonia and Barnett Shale. This could indicate that clay and biogenic quartz have a higher retention potential. Within Niobrara and Barnett Shale, samples from organic rich units have higher $(O_xN_y+N_y)/O_x$, N_2/N_1 and N_2O_1/N_1O_1 ratios. O_xN_y and N_y compounds might be preferentially retained in the source in comparison to O_x compounds, and compounds containing two nitrogen atoms are better retained than compounds containing one nitrogen atom. High variability in $(O_xN_y+N_y)/O_x$ values can be found between Barnett source and reservoir samples, while this variability is small within Niobrara sample set (Figure1). This could be due to more efficient secondary migration in carbonate rich Niobrara samples.

Within Niobrara Formation and Barnett Shale, samples from organic rich units have higher contribution from compounds with high DBE values and compounds in low carbon number range within a specific DBE class, especially in N_1O_1 compound class. High DBE values indicate high aromaticity and increased molecular size of compounds. Compounds in low carbon number range represent compounds with low alkylation grade and higher polarity in specific species. This fits to an observation of Mahlstedt et al (2016) that compounds with higher aromaticity and lower level of alkylation are preferentially retained. Higher contributions of N_1O_1 compounds with high DBE values ($DBE_{>9}$ N_1O_1 compounds) in Barnett and Posidonia Shale also argue for their increased retention potential compared to the Niobrara formation. This first insight into the (+)-APPI FT-ICR-MS data indicates their high potential to elucidate controlling effects of lithofacies on petroleum retention and migration in unconventional systems.

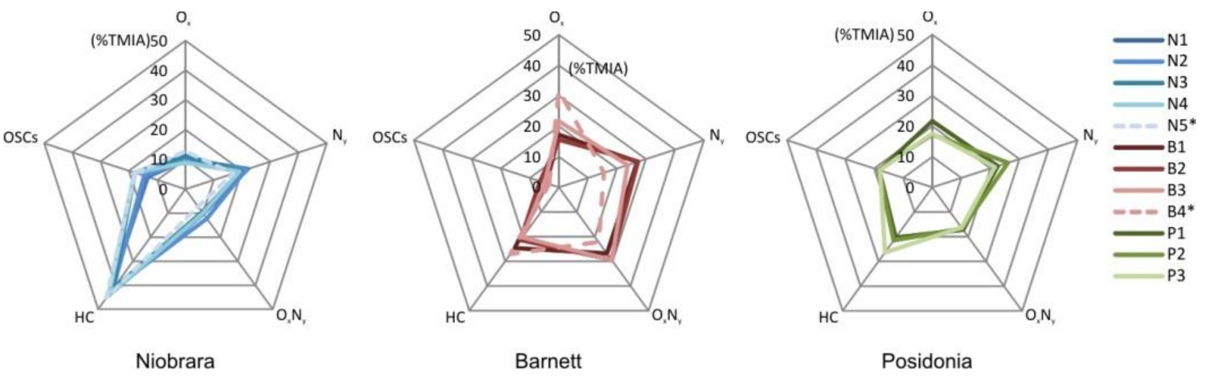

Figure 1 *Radar figures showing elemental class distributions of monoisotopic assigned peaks [%TMIA] in different samples. OSCs represent all sulphur containing elemental classes (S_z, O_xS_z, N_yS_z and $O_xN_yS_z$). "*" marks reservoir samples in Niobrara and Barnett sample sets.*

References

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