

## Molecular retention processes in source rocks: Can they explain fractionation during expulsion?

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Multi-component experimental generation patterns often disagree with observed reservoir composition, the latter being much less rich in aromatics and NSO compounds than the generated fluids. Adsorption has frequently been suggested to account for retention in coal, but the concepts brought forward to date are rather unspecific and not quantifiable. Absorption in the kerogen matrix based on polymer solution theory has been suggested for type I and II kerogen. This presentation looks at the interaction of adsorption in nanopores and polymer-solution-type absorption in source rocks and suggests quantifiable processes of fractionation.

Vitrinite is distinctly porous from the nano- to micrometer scale. Basic structural units (BSU) with widths around 1 nm and d002 spacing of 0.34 to 0.38 nm in bituminous coal and anthracite make up nanoporosity. Similarly, organic molecules may replace anorganic cations in inter-layer porosity of clays. If pore diameter approaches the diameter of molecules and the adsorption system is dominated by van der Waals forces, the Dubinin-Radushkevich (D-R) equation can be applied.

We used proprietary software PriMig to validate the processes, which to date reveals the following relationships: In coals, an absorption model based on Polymer Solution theory only, fails to eliminate heavy compounds sufficiently. A model based on D-R theory only leads to rather aromatic oils and condensates. However, a combination of adsorption- and absorption processes explains why coal expels gas, even if its chemical model may suggest generation of large amounts of C<sub>15+</sub> hydrocarbons. Coals with >5% porosity expel gas irrespective of composition of the original chemical generation model. Coals with initial potential around 300 mg/gTOC and with porosity <2% expel high-GOR petroleum fluids. GOR decreases with increasing initial potential.

The results obtained to date are encouraging and point in the right direction. Improved quantitative predictions need better knowledge of multi-component swelling ratios and adsorption, as well as temperature- and maturity-dependence of adsorption and solution systems. The presentation will show the newest available modelling examples of application and validation of the model.

## Fluid-rock interactions in petroleum reservoirs: Alkylphenols

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### Proxies for monitoring fluid-rock interactions

The interaction of petroleum compounds with mineral surfaces is one of the key mechanisms determining which phase, oil or water, wets mineral surfaces in petroleum reservoirs. Using a number of approaches we describe how polar surfactant molecules (i.e. alkylphenols) behave during crude oil / brine / rock interactions in petroleum reservoirs.

### Results and Discussion

A core-flood experiment was designed to monitor the chemical and physical changes during oil migration (Bennett et al., 2004). Wettability alteration shown by Environmental Scanning Electron Microscopy is consistent with changes in C<sub>0</sub>-C<sub>3</sub>-phenol distributions. In natural systems, alkylphenols display similar behaviour to those described from the core-flood. Molecular modelling experiments (van Duin and Larter, 2001) provide a fundamental explanation of wettability alteration observed during the core-flood. We propose that C<sub>0</sub>-C<sub>3</sub>-phenol serve as proxies for describing crude oil / brine / rock interactions in petroleum accumulations.

### Conclusions

The C<sub>0</sub>-C<sub>3</sub>-phenols represent an important class of surfactant molecules that can provide information regarding the nature of crude oil / brine / rock environment of petroleum reservoirs.

### References

- Bennett, B., Buckman, J.O., Bowler, B.F.J., and Larter, S.R. (2004), *Petroleum Geoscience* **10**, 271-277.  
van Duin A.C.T. and Larter S.R. (2001), *Organic Geochemistry* **32**, 143-150.