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GEOS4 Pioneer Service Project

ONSET

a Multiclient Study of Polar Compounds in Petroleum Systems

Flow Assurance, Production Allocation and Reservoir Heterogeneity are Key Issues to be Addressed

We offer rapid ultra-high resolution analysis and evaluation of **POLAR COMPOUNDS** utilising Fourier Transform Ion Cyclotron Resonance Mass Spectrometry.

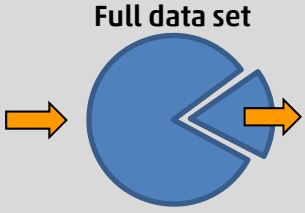
FT-ICR MS covers the widest molecular mass range from 50 to >10.000 atomic mass units/Dalton and is therefore a perfect tool for the characterization of polar compounds in complex mixtures occuring in crude oils, tar mats, shale extracts, bitumens, seeps, asphaltenes.

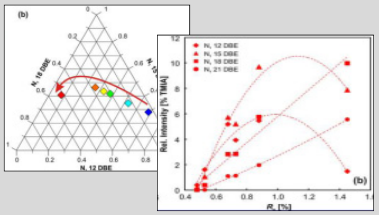
The ONSET Project

- Kicks off March 2016 with a minimum of four participants.
- Duration: 6 months
- Each company donates two samples to the consortium.
- Additional six samples are provided by GEOS4 at no extra costs.
- Mixed sources, produced versus in-place oil, tar mats, source and reservoir extracts can all be considered.
- Analysis mode is electrospray negative, targeting carbozoles (N_1), phenols (O_1), acids (O_2) and heteroatom combinations (N_1O_1, N_1O_2, N_1S_1).

Data

- Targeted data analysis.
- Data can be revisited for future interpretation.





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ONSET Project Deliverables

- Whole oils and whole reservoir core extracts will be analysed using FT-ICR MS in Electrospray negative ion mode.
- Compound classes coming under scrutiny are carbozoles (N_1), phenols (O_1), acids (O_2) and combinations (N_1O_1, N_1O_2, N_1S_1). In each case, the relative abundances of e.g. 1, 2, 3, 4, etc. ring systems and/ double bonds (as Double Bond Equivalents DBE), and the chain length distribution of aliphatic substituents for each DBE class will be quantified and the results interpreted.
- Additional major species, natural and anthropogenic, will be identified.
- The interpretation report will be accompanied by targeted data in tabular form, interpretation diagrams and geochemical indices.
- Influence of facies, maturity, retention, mixing and biodegradation on polar compound composition will be considered, in close cooperation with the sponsors.

Milestones

	2016											
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
FT-ICR MS analytics of samples												
Interpretation of dataset												
Report writing												
Workshop with participants												

Innovation Through Research

GEOS4 is one of the very few vendors worldwide to offer this specialised service to the industry. The company has established and continues to develop its state-of-the-art polar compound portfolio by means of its staff's published research, acquiring the necessary data from GFZ German Research Centre for Geosciences.

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ESI FT-ICR MS Plots Provided

Plot name	Parameters	Plot types	Peak selection (monoisotopic)
Elemental class distribution	Relative Intensity of elemental classes [%TMIA]	pie chart	all peaks
Compound class distribution	Relative Intensity of compound classes [%TMIA]	pie chart; bar chart	all compound classes >1%TMIA
Van-Krevelen diagram	H/C vs O/C	xy chart	all peaks OR selected compound classes
(pseudo) Van-Krevelen diagram	H/C vs N/C; H/C vs S/C	xy chart	all peaks OR selected compound classes
Kendrick mass defect diagram	KMD vs nominal mass; KMD vs carbon number	xy chart	all peaks OR selected compound classes
Double bond equivalent plot	DBE vs Carbon number; DBE vs. m/z	xy chart	selected compound classes
DBE class distribution	Relative Intensity of DBE classes [%TMIA]	bar chart	selected compound classes
Carbon number class distribution	Relative Intensity of carbon number classes [%TMIA]	bar chart	selected DBE classes (of a compound class)
Hexagonal Class Representation	Relative Intensity of elemental classes [%TMIA]	hexagon	all compound classes >1%TMIA
Maturity			
Mean DBE	Mean DBE of N_1 class [%TMIA] vs vitrinite reflectance	xy chart	N_1 class
N_1 20 DBE	Relative Intensity of N_1 DBE 20 class [%TMIA] vs vitrinite reflectance	xy chart	N_1 20 DBE class
N_1 ortho-peri annelated	Relative Intensity of N_1 DBE 17+20+23 class [%TMIA] vs vitrinite reflectance	xy chart	N_1 17, 20, 23 DBE classes
N_1 9, 12, 15 DBE	Relative Intensity of N_1 12, 15, 18 DBE classes [%TMIA]	ternary	N_1 9, 12, 15 DBE classes
N_1 17, 20, 23 DBE	Relative Intensity of N_1 17, 20, 23 DBE classes [%TMIA]	ternary	N_1 17, 20, 23 DBE classes
Chain length distribution	$C_{0\text{-}5}$, $C_{6\text{-}14}$ and C_{15+} compounds of selected DBE classes from N_1	ternary	N_1 selected DBE classes
Mixing			
Venn Diagram	All molecular formulas	overlapping circles	all peaks or compound classes
Biodegradation			
A/C ratio	Ratio of acyclic to 1-3-cyclic carboxylic acids vs. API gravity or TAN	xychart	O_2 compounds with DBE 1,2,3,4
Statistics			
PCA (Principal component analysis)	Molecular formula	xy chart	all peaks

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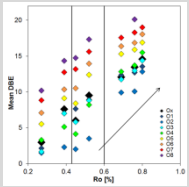

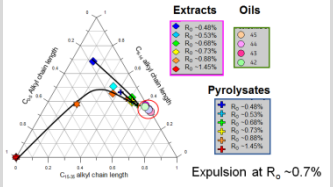

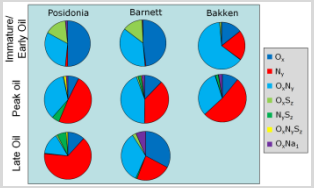

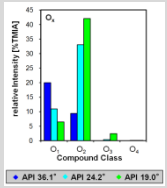

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