Beyond petroleomics – Petroleum geochemistry for the 21st Century

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Petroleum geochemistry has been driven by analytical developments since the development of gas chromatography in the 1950's and practical computerized GCMS technologies in the 1970's heralding, in the 70's and 80's, the development of practical biomarker technologies and most of the source rock facies and maturity molecular concepts that we still use today. Recent advances in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR-MS) technology now allow a more comprehensive analysis of polar constituents of fossil fuels. This new technology allows for the first time routine analysis of the broad range of complex polar compound mixtures that dominate source rock extracts and heavy oils.

In this study we will show the use of FTMS derived high molecular weight multi hetero component (HMWMH) complex compound class distributions to discriminate biodegraded oils from different source rocks from marine versus lacustrine systems and also differentiate oil charges from mixed facies marine source rocks. These new proxies are independent of microbial biodegradation alteration levels from Peters & Moldowan levels 0 to 8 (Peters and Moldowan, 1994) and show that it is likely that FTMS techniques and parameters may offer substantial advances over conventional GCMS based approaches to petroleum system characterisation. In addition, new insights into the compositional changes during *in situ* thermal recovery processes simulated in the lab under aquathermolysis and hydrotreating conditions will be shown.

The environmental impact of sewage effluent discharges in the Pracana River - Portugal

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The Pracana River is an important tributary of the Ocreza River. The Ocreza River is located in Central Portugal and has it source in an important Alpine chain called Gardunha. It starts at 1160 m altitude and stretches for 80 km until draining into the Tagus River. It has several creeks and tributaries along which there are several rural villages. The Pracana's waters has an important role by being abundantly used in agriculture, the main economic activity of these communities, and for human consumption. Characterization, monitorization and control of the impact due to several wastewaters treatment plants discharges on water quality is of crucial importance.

This paper focuses on the Proença-a-Nova wastewaters treatment plant, which discharges directly into the Freixada River, a Pracana's tributary. Twelve georeferenced water samples were collected between the sewage effluent discharge and the Pracana river confluence. Secondary inflows were identified and water samples collected downstream at approximately equal distances. The core of our study is the hydrological year of 2010. Sampling campaigns were conducted during three different periods: rainy winter (January), intermediate conditions (March) and dry season (June). The following chemical parameters were analyzed: biochemical oxygen demand (BOD), dissolved oxygen concentration (DO), dry residue, P_{total}, N_{total}; pH, temperature and microbiological parameters. The dissolved oxygen concentration (DO), biochemical oxygen demand (BOD) and the microbiological parameters were used as indicators for the presence of organic matter in the body of water, and as parameters for evaluating the environmental pollution.

The pollution simulation in the Pracana river was performed by a coupled hydrodynamic and water dispersion model. A water quality model was constructed applying to QUAL2kw software. The simulation results are consistent with field observations and demonstrate that the model has been correctly calibrated. The model is suitable for evaluating the environmental impact of wastewaters plant discharges on the Pracana River, allowing feasibility studies of different treatment schemes and the development of specific monitoring activities.