

Asphaltene present in crude oils of Alagoas sub-basin studied by ESI FT-ICR MS

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Problems associated with asphaltene precipitation and deposition have been widely reported in the petroleum production and processing industry. Asphaltene is the most polar fraction in crude oil, with heavy N, S, O-containing molecules (molecular weight >500), insoluble in n-pentane (or n-heptane) and with average molecular mass of asphaltenes of <1,000 Da. Electrospray (ESI) selectively ionizes the polar compounds and FT-ICR MS provides the high resolution (> 100,000) and high mass accuracy (< 1 ppm) needed to resolve and identify a complex mixture as asphaltene. This paper compares the composition of the asphaltene of 7 crude oils from Alagoas sub-Basin.

The asphaltenes present in the oils (PMAS, PAAS, PCAS, PNAS, PDAS, FUBAS and FUAAS), were precipitate in n-pentano (2 x 6 mL) and after the centrifugation (2 x 2500 RPM, 20 min), the precipitate was dissolved in DCM (1 mL) and 2 µL of a 1% aqueous solution of ammonium hydroxide was added to form the negative ions.

Using microelectrospray ionization FT-ICR MS mass spectrometry (ESI FT-ICR MS), it is possible to identify similarities and differences between the asphaltenes samples for the 7 oils. The graphic images, compiled with software PetroMS, (Fig. 1) show that compounds with nitrogen N, O, and S were identified in different relative proportions in the samples. Asphaltenes samples showing the same classes, does not mean they contain the same types of compounds. The Fig. 2 represents a two DBE plots for the O₂ compounds identified from PAAS and PCAS crude oil, and it exposed compositional differences in the acid species and showed that the PAAS sample, despite containing the same O₂ percentage that PCAS, contained a O₂ class composed of lower ring plus double bond compared PCAS. Similar differences were observed also in others oils and these differences, based in its polar composition, could give clues to oil origin.

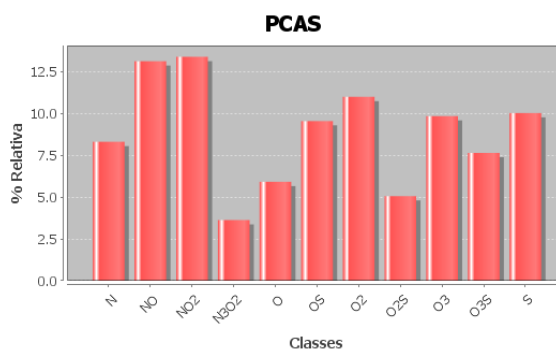


Fig. 1. Relative abundances for various compound classes in the negative-ion ESI FT-ICR mass spectra of the asphaltenes to the crude oil PCAS.

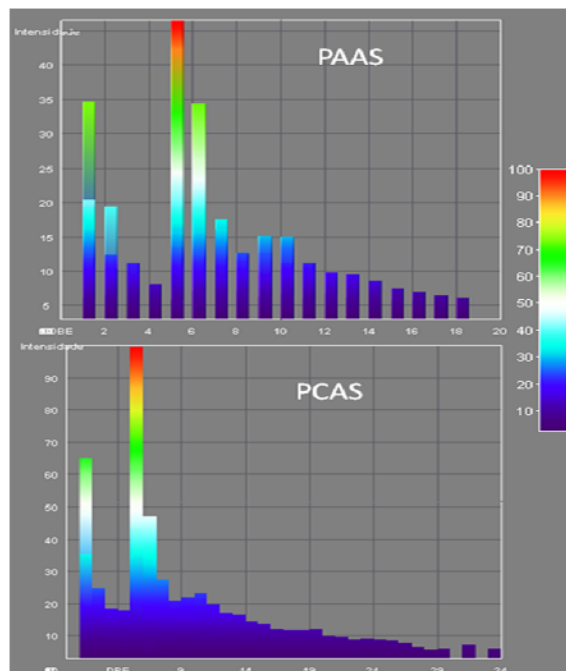


Fig. 2. Type distribution for the O₂ compounds identified in the negative ion ESI FT-ICR mass spectra of two oils from Alagoas sub-basin. Note that there are in the PCAS oil O₂ compounds with distribution range 1 < DBE < 34 shows that O₂ class is more aromatic in PCAS than PAAS.