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Molelcular dynamics simulations techniques applied to study asphaltenes' molecular cartography and aggregation properties in crude oil

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The challenges faced by the oil industries comprise the comprehension of the physical-chemical behaviour of the heavy-weight phases. These phases have a high tendency to aggregate and this is mainly due to asphaltene molecules which constitution are still unclear. The molecular cartography of this phase is one of the driving forces of this behaviour and the structure-property relation is a key point to the development of refining techniques displaying more performance. In this presentation, the aggregation of asphaltene molecules is studied upon the light of their molecular cartography, thermodynamic conditions and dimensionality screened by several molecular simulations techniques, in particular, density functional theory and molecular dynamics simulations.The effect of the heteroatom substitution and the molecular architecture on the aggregation pattern and energies of asphaltenes nano-aggregates in various thermodynamics conditions will be presented. Our group showed that the heteroatom substitution on the aromatic core does not change the type of the nano-aggregation but changes considerably the interaction energies. Moreover, we presented arguments towards the role of these heteroatoms on the shape of the aggregates when they are found in the lateral chains. Besides this, we also showed that the aggregation strength depends strongly on the shape of the aromatic core. In order to get closer to the real complexity of heavy-oil phases, we recently considered the effect induced by porphyrins on the nano-aggregation phenomenon. These results, give us a general overview on which are the factor that have the strongest impact on this physical-chemical behaviour of heavy-oil phases.

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