

## Insight into asphaltene nano-aggregate structure inferred by small angle neutron and X-Ray scattering

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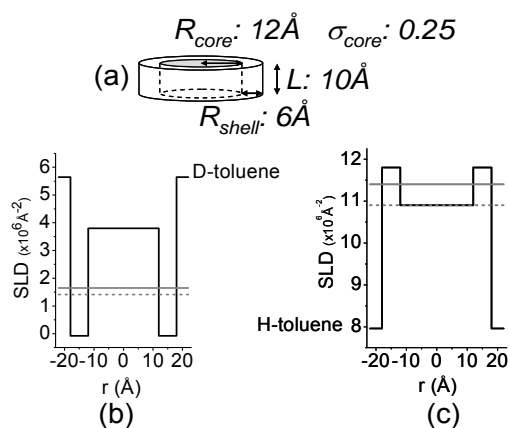
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Aggregation of asphaltene in solutions or crude oils is well established and the primary aggregation leading to the "modified Yen Model" has been reviewed recently [1]. The emerging picture is a stacking of few "continental" molecules giving rise to so called 2 nm nano-aggregates whose internal part is mostly aromatic whereas peripheral counterpart is rather aliphatic. The small angle neutron or X-Ray scattering (SAN(X)S) response give much larger sizes (5-10 nm) and various form factors (spheres, discs,...) have been suggested to account for data. We recently propose a structural model taking into account these two typical sizes, namely a mass fractal model (cluster of nano-aggregates) which allows viscosity of asphaltene solution to be fully predicted [2]. We focus here on small length scale of SAN(X)S curves which gives access to nano-aggregate structure.

We take advantage of complementary properties of neutrons and X-Ray with respect to scattering length density (SLD) of asphaltene: the intensities measured using neutrons or X-Rays of the same asphaltene solution doesn't scale with mean contrast in the high  $q$  domain. This discrepancy is accounted by regions of different SLD and consequently different composition [3].

Thanks to precise absolute measurements at large  $q$  values, the data are fitted to Form Factors of core-shell spheres or cylinders. The retained solution is the one which i/ maximizes the fitted  $q$  range, ii/ gives the same core and shell dimensions for neutrons or X-Rays, iii/ gives the calculated SLD equals to the one deduced from composition and density of asphaltene, both for neutrons and X-Rays. These conditions, which are very restrictive, ensure the quasi uniqueness of the solution. It must be pointed out that some core polydispersity has to be introduced in order to nicely fit the scattering data

The nano-aggregate picture which comes from scattering spectra acquired at moderate concentration ( $\approx 5\text{g/l}$ ) of asphaltene in toluene is shown on Figure 1.



**Fig. 1.** Geometrical characteristics of nano-aggregates (a) and the corresponding SLD profile for neutron (b) and X-Ray (c) scattering. Mean SLD (full line) deduced from SLD profile are compared to those calculated from asphaltene composition and density (dotted line).

The core and shell SLD values both for neutrons and X-Rays are found consistent with respectively aromatic and aliphatic compositions. Relevance of this model in terms of shape, dimensions of core and shell, core polydispersity, radius of giration, mass, aggregation number, diffusion coefficient, will be discussed. This description at intermediate length scale between the molecular and the cluster one gives new clues in the asphaltene structure puzzle.

### References

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