

## On the equilibrium shapes of asphaltenes in solvents

Pawel Peczak

*ExxonMobil Research & Engineering, 1545 Route 22 East Annandale, NJ 08801-0998)*  
(\* corresponding author: [pawel.k.peczak@exxonmobil.com](mailto:pawel.k.peczak@exxonmobil.com))

Deposition of hydrocarbon films on the walls of pipes or vessels is a source of long-standing operation problems in the petroleum industry. Asphaltenes represent a solubility class that is well known to exhibit this phenomenon. In order to prevent the deposition process, more needs to be known about their behavior in the oil mixtures. Unfortunately, due to the molecular diversity of petroleum, the nature of interaction between asphaltenes and other molecules, either in the liquid state or those in the solid walls, is still a matter of debate. In particular, the nature of the asphaltene-asphaltene interaction has been a subject of long-standing controversy. Several recent reports have suggested that asphaltenes self-associate in stacked nano-structures. However, the quantitative description of the asphaltene-oil interactions that is consistent with this picture is far from being achieved. Even a much simpler problem, that of the shape of asphaltene molecules in solvents of different quality has yet to be fully addressed.

Toward that end, we have implemented a lattice-based model of the petroleum matrix that combines a conceptually simple geometric description with a systematic analytical analysis of asphaltene-oil interaction. The asphaltenes are modeled as pseudo-molecules built of two kinds of segments. The center of the molecule is represented with an aromatic core while the side-chains have a typical aliphatic character. In the dilute regime, the molecules are separated from each other by the "sea" of solvent-like segments of a uniform solubility. Using a simple yet robust assumption about the nature of segment-segment interaction [1], we have obtained the solvation energy of asphaltenes of a given topological class in different solvents. By comparing the solvation energies of all possible configurations, we have found the most likely equilibrium shape for each class. The results help to understand why asphaltenes stick so readily to solid surfaces. We have also suggested that the often-invoked picture of asphaltene nano-stacks may be inaccurate.

### References

- [1] J. Israelachvili, "Intermolecular & Surface Forces", Academic Press - Elsevier (1991) 2nd Edition