

Comparative Study of Asphaltene-Inhibitor Interactions by Density Functional Theory

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INTRODUCTION

Asphaltenes represent major technical problems and challenges of the petroleum industry, since they are responsible for causing major losses in all effective methods of prevention and remediation of this problem is the use of asphaltene inhibitors that prevent the aggregation of asphaltene molecules². Molecular modeling can play an important role in the investigation of association phenomena of asphaltenes³ but the majority of the standard semiempirical, density functional theory (DFT) and ab initio methods does not properly account for the dispersion term⁴.

METHODS

Two structures of asphaltenes (BB and BD) and two potential inhibitor molecules, p-nonylphenol and cardanol, were used for computational simulations. Docking between the most stable structures of each asphaltene and inhibitor molecules was carried out and conformational analysis of each asphaltene-inhibitor structure was made by molecular dynamics using the COMPASS force field. The asphaltene-inhibitor interaction was calculated by Density Functional Theory (DFT) using the SVWN and ω B97X-D functional. The efficiency of an inhibitor of asphaltene deposition, p-nonylphenol, were evaluated and compared against an inhibitor synthesized from a renewable source (cardanol).

RESULTS AND DISCUSSION

The interaction energy calculated by SVWN and ω B97X-D functionals to asphaltene-inhibitor system can be seen in the Table 1.

Table 1. ΔE (kcal/mol) obtained for asphaltene-inhibitor interactions.

Interaction	SVWN	ω B97X-D
BB-p-nonylphenol	-20.2	-29.9
BD-p-nonylphenol	-25.8	-36.9

The Table 1 shows that calculated interaction energies to BD-p-nonylphenol are larger than BB-p-nonylphenol. Calculated energies by the local exchange-correlation functional SVWN are larger than calculated ones by functional ω B97X-D that has atom-atom dispersion corrections. These are important results because normally functional with local exchange-correlation overestimate binding energies of weakly bound systems. The calculations to asphaltene-cardanol structure are being realized.

CONCLUSIONS

The simulations suggest that the interaction of the p-nonylphenol with BD- asphaltenes is better than BB-asphaltenes, for both functional studied, although the energies are relatively close.

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