Theoretical Study of the Interaction Between Asphaltenes and Methane Hydrates

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Semiempirical molecular dynamics (MD) calculations, at the NVE ensemble and at temperatures of 0, 3 and 5 °C with the compass force field, were carried out to investigate the effect on the aggregation of methane hydrate crystallites due to the presence of asphaltenes. Methane hydrates crystallite cumulus with the 5^{12} structure and the $5^{12}6^2$ structure were considered. Different validated structures of asphaltenes were also considered were the effect of their polydispersity is analysed.[1, 2, 3, 4, 5] It is found that the presence of asphaltenes disrupts the aggregation of the methane hydrates due to interactions, mainly via hydrogen bonds, between the asphaltenes and the methane hydrate crystallites.

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