Coarse grain models for molecules with fuzzed-rings fragments: the case of kerogens

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ABSTRACT

Organic molecules consisting, among others, of groups of fused rings are widespread in nature and are found in many processes such as shale gas extraction (kerogen)[1] and crude oil processing (asphaltene)[2]. In this work, we focus on developing models for the coarse-grained (CG) description of kerogen structures of variable type and thermal maturation using the MARTINI force field (FF)[3] approach. This method has the advantage of combining top-down and bottom-up modeling techniques, with the parameters optimized using macroscopic attributes and structural data produced by all atom simulations. First, we verified that MARTINI FF reproduces the experimental bulk densities of stiff, tiny compounds with good accuracy. These compounds are similar to the molecular fragments present in kerogens. Then, CG models for kerogen were developed and used to create configurations with structural properties that are similar to those of their counterparts in all atom representations. Our objective is to apply molecular modeling techniques to realistically describe larger and more complex control volumes of a shale field and investigate gas sorption and diffusion within them [4-6].

KEYWORDS: molecular modeling, coarse grain models, kerogen.

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