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Superamolecular Chemistry and Packing of FAMEs in the Liquid Phase for Optimization of Combustion and Emission

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Abstract : Supramolecular chemistry refers to the domain of chemistry beyond that of molecules and focuses on the chemical systems made up of a discrete number of assembled molecular sub units or components. Biodiesel components self arrangements is closely related/affect their physical properties in combustion systems and emission. Due to technological difficulties, knowledge regarding the molecular packing of FAMEs (biodiesel) in the liquid phase is limited. Spectral tools such as X-ray and NMR are known to provide evidences related to molecular structure organization. Recently, it was reported by our research group that using 1H Time Domain NMR methodology based on relaxation time and self diffusion coefficients, FAMEs clusters with different motilities can be accurately studied in the liquid phase. Head to head dimarization with quasi-smectic clusters organization, based on molecular motion analysis, was clearly demonstrated. These findings about the assembly/packing of the FAME components are directly associated with fluidity/viscosity of the biodiesel. Furthermore, these findings may provide information of micro/nano-particles that are formed in the delivery and injection system of various combustion systems (affected by thermodynamic conditions). Various relevant parameters to combustion such as: distillation/Liquid Gas phase transition, cetane number/ignition delay, shoot, oxidation/NOX emission maybe predicted. These data may open the window for further optimization of FAME/diesel mixture in terms of combustion and emission.

Keywords : supermolecular chemistry, FAMEs, liquid phase, fluidity, LF-NMR
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