THERMODYNAMIC ANALYSIS BY BIODIESEL AND DIESEL DFT METHOD

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This work will make a thermodynamic analysis of the combustion of its majority molecules in average percentages contained in the main available oleaginous ones and compare them with the majority combustion of the fossil diesel derived and checking which had better efficiency in energy, Gibbs energy, specific heat and enthalpy. To enable an analysis of the thermodynamic properties of diesel as well as of biodiesel through theoretical calculations using the Density Functional Theory (DFT) method as well as the simulations written through the Gaussian 09W and Hyperchem 7.5 software. It will be used to perform molecular geometry optimization calculations using the DFT and the polarizable continuous model (PCM) with hybrid function B3LYP. Thus the temperatures with both Biodiesel and Diesel will be in the range of 0.5K - 1500K and under the pressure of 1atm. At first, optimizations were made by DFT and PM3 methods demonstrating agreement of results at first as exposed in fig. 1 to 20 similar molecules and the results were compared energetically and structurally using the parameterization of the functions that makes it possible to relate such simulations to analytically search solvated systems of each biodiesel and diesel major component, however, conformational analysis, optimization of molecular geometry and frequency calculations. They will enable this work to obtain physical properties preponderant to the chemical spontaneity and coexistent calorific power in majority molecules of biodiesel and diesel in the gas phase. The objective is to discover thermodynamic properties that will allow its characterization at the molecular level, thus allowing to verify the common characteristics and to design new combinations of diesel and biodiesel. At the end of the work a weighted average of the Diesel and Biodiesel molecules that were dosed in different percentage rates was analyzed, analyzing their biodegradable structures, we verified that it is miscible with the diesel in any proportion, leading to the diesel / biodiesel binary mixture.

Keywords: DFT; Diesel; Biodiesel.

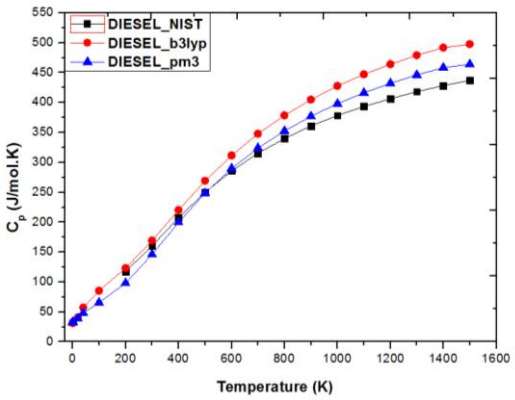

Figure 1 - Specific heat at constant pressure versus temperature.