THERMODYNAMICS CHARACTERIZATION OF BIODIESEL ADDITIVES AND THEIR EFFECTS IN THE B100, B8 AND B20 BLENDS

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Abstract

Recently, due to price increases of oil, limited resources of fossil oil and the environmental worries, there is been a renewed focus on vegetable oil and animal fat to produce biodiesel. The fuel called renewable is included in the area of alternative energies, which come from natural resources having regeneration capacity, that is, it is not possible to establish a temporal end to its usage. However, Biodiesel has some practical difficulties to its usage and, between them, we remark in this study the low stability oxidative, the existence of high pour point and degradation by microorganisms. Classically, these difficulties are attenuated with usage of additive to the fuel and in this work, we try to analyze what are the effects of the presence of these additives on soy Biodiesel, mainly which thermodynamics changes that they are capable to introduce in the fuel. In this study we use Pyrogallol, gallic acid, polymethacrylate in the pure Biodiesel (B100), 8% diesel and 20% biodiesel (B8 and B20). We made some simulation of conformational analysis and molecular geometric optimization on Hyperchem 8.0 and the second geometric optimization using DFT method and frequency calculation both under B3LYP functional and 6-311++g(d,p) base. Finally we apply rules of mass fraction of the components to analyze the effect of the additions. The results show that, in the employee concentration, the use of these additives virtually does not induce changes in the thermodynamics parameters of the three fuels (B8, B20 e B100), not even under the "additive packs" technique. In this way the additives only act on the their functions.