Mathematical Approach to Compute the Molecular Composition of HTL-derived Renewable Crude Oil

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Abstract

To assess the techno-economic screening of HTL oil for various feedstock, it is crucial to have information on molecular composition of the feed and products. There are limitations of existing analytical methods to identify and quantify all the molecules present in the bio-fuel. Therefore, there is a need to find alternate ways to quantify the molecular composition of feed and expected products. The modelling work on bio-oil is developed based on a mathematical approach using simple analytical results like CHNO along with structural analysis of oil like FTIR, NMR analysis for HTL derived oil from microalgae. This mathematical framework is further extended to predict the molecular composition of HTL-oil obtained from feedstocks like mixed plastic waste, sludge etc. A multi-dimensional molecular matrix is developed based on the distributions of side chains, aromatic rings, and olefinic carbon on top of core molecules. Optimum parameters are found using appropriate optimization algorithms.

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