GC and GC×GC based approaches for the molecular characterization of complex matrices related to alternative energy sources

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The continuing global energy demand makes biomass feedstock one of the promising resources to cope with more sustainable and greener energy challenges and reduce the dependency on fossil-based energy sources. Animal fats as well as vegetable oils, and tomorrow biomass-pyrolysis oils, represent interesting new sources to produce biofuels. In the same way, the conversation of the large amount of plastic residue by mechanical or chemical techniques, such as pyrolysis, can also reach the needs for circular economy. Regarding the composition, besides triacylglycerols, biomasses feedstocks contain a wide range of other contaminants which can affect the technical properties of the raw fat feedstock. For example, higher acid content can cause severe corrosion in the fuel supply system of engines, impacting the catalytic transesterification process, while the possible condensation of aldehydes and ketones could lead to the formation of gums [1-3]. Coming back to plastic pyrolysis oil, even though their chemical composition shows similarities with fossil-based hydrocarbons fluids/cuts, e.g. PIONA related compounds, some N- and S- or O-containing compounds can be found and could be related to adverse qualities of the final product. In both feedstock cases, an exhaustive characterization by GC and GC×GC hyphenated with mass spectrometry of these compounds was made and is fundamental for performing the most appropriate pretreatment. In addition to these targeted impurities, molecule family type speciation was performed as it is key for the molecular modeling of biofuel properties. Despite this powerful GC×GC-MS based approaches, there is still a lack in the detection mode for the detailed and quantitative characterization of oxygenated compounds, especially when biomasses biofuel is the objective. For this reason, a new GC detector able to provide compound-independent quantification of C, H, N and S in complex samples was developed in the past years thanks to a collaboration between the universities of Oviedo (Spain) and Pau (France) and TotalEnergies [4]. A commercial GC-MS was modified by using a combustion interface between the GC and the final MS analysis in order to detect every organic compound present as volatile species formed during their combustion (CO2, H2O, NOx, SOx). It this therefore possible to achieve a species-independent generic and simultaneous quantification of C, H, N and S. Importantly, GC-combustion-MS can be used as well for the detection of oxygen if enriched 18O-oxygen is used for the combustion (WO2017/114654 patent)

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