Molecular characterization of new renewable feedstocks by multi-scale analysis using gas chromatography, mass spectrometry and an oxygen selective detector

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Alternatives to fossil fuels have been at the forefront of scientific research for many years. Detailed molecular characterization of new feedstocks such as pyrolysis oil from biomass, recycled plastics or from used wind blades is therefore of prime importance for better understanding and predicting the macroscopic behavior of these new types of materials. It is necessary to understand their faith in the part of the energy transition. These feedstocks are made of complex chemical mixtures that require multi-scale analysis to be properly characterized at the molecular scale. Several analytical techniques are currently employed for this very purpose. The volatile fraction of the samples can be analyzed by gas chromatography (GC) hyphenated to mass spectrometry to identify the unknown compounds.

In comparison to classical fossil fuels, the diversity of the chemical classes present in such samples is very large and comprehensive two-dimensional gas chromatography coupled to mass spectrometry (GCxGC-MS) was successfully used in an earlier study [1,2]. A GCxGC system operating with a reverse column set has been investigated in the present study to separate, identify, and quantify compounds present in hydrotreated vegetable oil to be used to produce sustainable aviation fuel (SAF).

Next to MS, heteroatom-specific detectors such as NCD and SCD can also be coupled to the chromatographic separation to gain additional valuable informations. Because some compounds, like oxygenated molecules, can significantly impact the macromolecular properties of the alternative fuel, with a direct impact on its properties and usability, the need for clear understanding of oxygen-bearing compounds present in pyrolysis oil is a major goal [3]. However, quantifying and identifying oxygenated molecules is a major limitation due to the lack of oxygen-specific detectors suitable for this purpose.

To address this, a new type of oxygen-specific detector capable to identify and quantify molecules without the use of any standards was recently developed [4] and used in this study. In addition to the characterization of oxygen-containing molecules, this new GC detector can also detect and quantify carbon, nitrogen and sulfur by considering their volatile forms: CO_2, NO_x and SO_x [5].

This multi-scale analytical approach involving GCxGC and various type of detectors appears to be valuable for the characterization of new feedstocks and to enhance our ability to adapt the related industrial processes in order to produce high-value products.

References:

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