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Integrated analytical workflow with ultra-high-resolution mass spectrometry for precise molecular profiling of complex waste- and biorefinery streams

PEDRO CASTANO

King Abdullah University of Science and Technology

Heterogeneous catalytic conversions drive ~80% of conventional refinery processes [1], yet comprehensive compositional analysis remains challenging. Understanding reaction mechanisms and optimizing catalyst design requires detailed molecular insights, particularly for unconventional feedstocks [2]. This study integrates ultra-high-resolution mass spectrometry (UHR-MS) into analytical workflows, bridging qualitative molecular data with quasi-quantitative insights. This work addresses key analytical challenges in integrating advanced techniques into traditional workflows to study compositional changes and reaction networks in unconventional feedstocks, proposing methods for translating qualitative molecular information into a quasi-quantitative description.

First, we employ a multi-technique approach—gas chromatography-mass spectrometry (GC-MS), bulk elemental analysis, and Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS)—to investigate heteroatom removal in vacuum gas oil (VGO) blends with oxygenated plastics (e.g., PMMA, PET). Results reveal a direct correlation between polymer structure (linear vs. aromatic) and heteroatom removal efficiency [3,4]. Next, we extend this framework to VGO-pyrolysis wax blends from HDPE, transforming qualitative FT-ICR MS data into a quasi-quantitative distribution. Using simulated distillation results to define compositional boundaries, we integrate data from GC-FID, GC-MS, and APPI(+) FT-ICR MS. The developed workflow harmonizes diverse analytical inputs, yielding comprehensive datasets applicable to continuous-lumping kinetics. We apply this quasi-quantitative approach to bio-oils, addressing challenges like the lack of commercial internal standards. We examine the effects of water content and ionization source on method applicability across bio-oils with varying hydrodeoxygenation (HDO) levels. Findings underscore the relevance and limitations of extending petroleum-derived analytical methodologies to oxygen-rich bio-based feedstocks.

In conclusion, this work advances UHR-MS applications in sustainable feedstock processing by refining FT-ICR MS quantification strategies, integrating complementary analytical techniques, and leveraging kinetic modeling. These developments contribute to expanding Petroleomics into the emerging field of Wasteomics.

REFERENCES

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