Using high resolution mass spectrometry to study fuel chemistry

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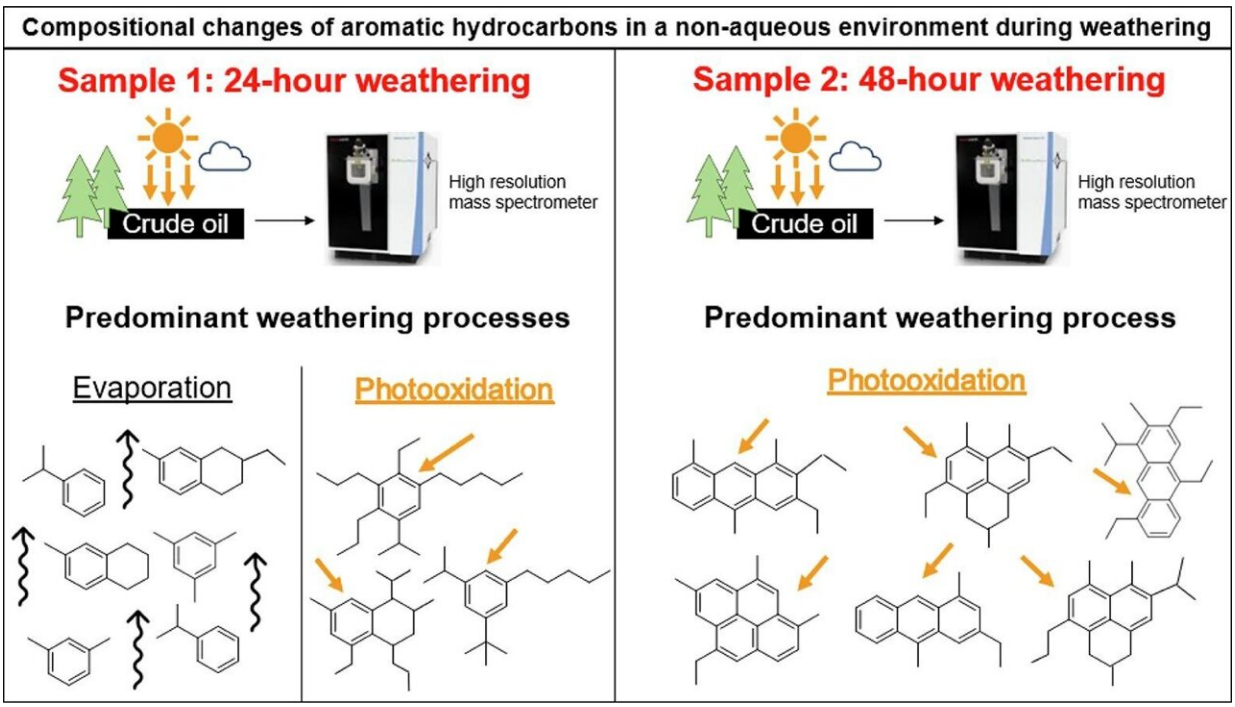

Credit: *Fuel* (2024). DOI: 10.1016/j.fuel.2024.132379

U.S. Naval Research Laboratory researcher Mark Romanczyk, Ph.D., developed new analytical methods to rapidly analyze fuels and complex petroleum products by using high-resolution mass spectrometry.

The approaches Romanczyk utilized enable highly detailed qualitative analysis of complex mixtures in minutes. One recent method facilitated

the investigation of chemical changes that occurred in weathered crude oil in terrestrial environments. Several of the methods were recently published in the science journal *Fuel*.

"Despite the accidental rise of oil spilled onto landmasses, less research has been dedicated to evaluating the compositional changes/fate of oil prior to its introduction into bodies of water" said Romanczyk. "The lack of information affords an opportunity to investigate and qualitatively characterize oil as a function of weathering time in the absence of an aqueous environment. These studies may provide highly useful information for oil spill cleanup and exposure concerns."

Upon direct sun exposure, the lightest aromatic hydrocarbons (i.e., alkylbenzenes, alkyltetralins with total carbons of approximately twelve) in the crude oil evolved in the first 24 hours of weathering. After 24 hours, a thin film formed on the surface trapping the lightest aromatic hydrocarbons where the overall composition remained unchanged.

However, the heaviest aromatic hydrocarbons (i.e., naphthalenes, anthracenes) showed evidence of photooxidation, despite film formation. The results demonstrate that the compositional changes of oil in a terrestrial environment may differ from that of an aquatic environment as wave action will likely stir the oil, preventing film formation.

Additional methods have been used to detect and characterize heteroatom-containing compounds (HCCs) in fuels. HCCs are a concern for fuel stability as they initiate adverse chemical reactions. The novel methods discovered new classes of HCCs not previously documented and aid in linking the composition of fuel to performance and properties.

"The approaches Mark and his colleagues are developing enable highly detailed analysis of fuel composition in minutes," said Kevin J. Johnson,

Ph.D., head, Navy Technology Center for Safety and Survivability. "I think this is going to lead to significant advancements in the near future in how we formulate and handle fuels in the Navy and Department of Defense."

Currently, Romanczyk is developing novel links between fuel compositions and stability properties and analytical techniques that detect PFAS (Per- and polyfluoroalkyl substances) at the parts per billion level. He also studies the weathering of crude oil.

More information: Mark Romanczyk et al, Compositional analysis and fate of aromatic hydrocarbons in weathered crude oil in a non-aqueous environment by using a high-resolution orbitrap mass spectrometer, *Fuel* (2024). DOI: 10.1016/j.fuel.2024.132379

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