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Compositional and Structural Analysis of Scrubber Discharge Water from a Ship Engine Using Liquid Chromatography and Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry

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Despite its crucial role in global trade, shipping significantly contributes to environmental pollution by emitting greenhouse gases and pollutants like nitrogen oxides, sulfur oxides, and particulate matter. To mitigate the harmful effects of ship emissions, the International Maritime Organization (IMO) has implemented a global limit on the sulfur content in marine fuels and introduced sulfur emission control areas (SECA). To comply with SOx emission regulations, ships can either operate on low-sulfur fuel oils or utilize alternative methods such as exhaust gas cleaning systems, commonly known as 'scrubbers'. Recent studies have shown that scrubber discharge water negatively impacts the aquatic environment and exhibits toxic effects on marine organisms. [1] While particle numbers are reduced by 40 % [2], research on the molecular composition of scrubber water and its environmental fate remains limited.

This study investigates the chemical composition of scrubber discharge water from a research ship engine, as well as its photochemical transformation products. Therefore, a laboratory photo-aging setup was used to simulate natural aging processes and evaluate both primary and aged scrubber water discharges. For desalting and enrichment, aqueous samples were subjected to a preconditioned solid-phase extraction (SPE) cartridge and subsequently eluted with methanol. Extracts were analyzed by direct infusion high-resolution mass spectrometry using an electrospray ionization source (ESI FT-ICR MS, 7 T, University of Rostock) to characterize the polar fraction of scrubber discharge water. Additionally, liquid chromatography hyphenated with 21 T FT-ICR MS was employed to reduce ionization suppression and introduce an additional separation dimension. The 21 T FT-ICR MS platform at the National High Magnetic Field Laboratory (NHMFL) provides ultra-high-resolution broadband acquisition at high scan frequencies, maintaining the full chromatographic resolution of advanced HPLC systems.

Ultra-high-resolution mass spectrometric measurements revealed a high molecular complexity of scrubber discharge water, with numerous resolved signals detected in a single liquid chromatography scan. A diverse range of oxygenated compound classes was identified, including species containing up to two sulfur atoms and over ten oxygen atoms. These compounds exhibited a broad aromaticity spectrum, with double bond equivalents (DBE) ranging from naphthenic to polycyclic aromatic moieties. The findings indicate that variations in engine operating conditions significantly impact the elemental composition of scrubber water. Laboratory photo-aging of scrubber water revealed compound class-specific transformations dependent on irradiation time, along with a general increase in highly oxygenated species. These transformations alter the chemical nature of scrubber water, highlighting potential risks related to environmental persistence and ecotoxicity in marine systems.

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