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AEROSOLOMICS FOR MARITIME EMISSIONS AND ENGINE DECARBONIZATION: FTMS FINGERPRINTS OF AMMONIA DUAL-FUEL EXHAUST AND WET-SCRUBBER DISCHARGES

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Maritime combustion remains a major source of particle- and heteroatom-rich emissions. Wet scrubbers can reduce particle numbers (reported reductions on the order of ~40%), but open-loop operation may relocate complex organic pollution from the atmosphere into the ocean as sensitive ecosystem. In parallel, ammonia is gaining attention as a carbon-free energy carrier; however, dual-fuel ammonia–diesel operation may alter emission chemistry in ways not captured by regulated metrics (NO_x, NH_3 slip, PM mass). These actions, likely resulting in emerging molecular repositories, motivate in-depth chemical characterization.
Two complementary aerosolomics workflows were applied. (I) Scrubber discharge waters were sampled and subjected to laboratory photo-aging. Methanol eluates after solid phase extraction were analyzed by 7 T ESI FT-ICR MS with MS/MS; LC hyphenation (including 21 T FT-ICR MS) preserved chromatographic resolution while reducing ionization suppression, and TIMS-ToF provided collision cross section (CCS) information. (II) A single-cylinder research engine was operated at 50/75/100% load (IMEP 10/15/20 bar) at ammonia energy shares up to 95%, with and without aftertreatment. Gas-phase aromatics were profiled online by laser-based photoionization MS at 248 and 266 nm (REMPI); particle emissions were collected on quartz fibre filters, extracted (MeOH/DCM 1:1), and analyzed by direct-infusion 7 T FT-ICR MS using (±)ESI/APPI, complemented by LC-HR-ToF-MS/MS and TIMS-ToF for isomer resolution and CCS validation.
Scrubber waters exhibited extreme chemical complexity, with several hundred resolved signals in a single LC scan. Oxygenated formula families included species with up to three sulfur atoms and over 10 oxygen atoms and spanned a broad aromaticity/DBE range from naphthenic to polycyclic aromatic motifs. Photo-aging increased oxygen content and functionalization, while CCS profiling separated isomeric/isobaric clusters associated with sulfur incorporation and oxygenation, consistent with substantial chemical transformation driven by operating conditions and secondary oxidative processing. For ammonia co-combustion, REMPI spectra at 15 bar IMEP were highly similar across ammonia shares, with no systematic shift toward lower *m/z* and no enrichment at odd nominal *m/z*. In contrast, FT-ICR MS of filter extracts assigned thousands of particulate-phase features, including abundant N/O-rich classes (up to N_4 and O_{10}) spanning wide DBE ranges; signals consistent with imidazole- and pyrazole-like motifs and multiple LC peaks per formula indicated pronounced isomeric complexity.
FTMS-based aerosolomics provides molecular metrics for maritime engines and decarbonization trade-offs: gas-phase aromatic fingerprints can remain comparatively stable while particle-phase chemistry diversifies strongly, and scrubber deployment can relocate complex oxygenated (including organosulfur) mixtures into the aquatic environment, motivating molecular-level assessment of persistence, reactivity, and toxicity beyond bulk compliance indicators.