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Legacy herbicides modulate nitrite partitioning and nitrogen retention during nitrate reduction in anoxic subsurface systems

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Diffuse agricultural pollution has generated persistent co-occurrence of nutrients and organic contaminants in soils and aquifers. Decades after regulatory restrictions, legacy pesticides such as atrazine and their transformation products remain widely detected, reflecting molecular stability and slow subsurface renewal. These environments function as long-term biogeochemical reactors where historical inputs continue to modulate redox dynamics and nitrogen cycling.

In anoxic subsurface systems, nitrate reduction initiates a branched reaction network structured around nitrite, a central intermediate whose partitioning governs nitrogen retention and versus redistribution.

We examined how structurally related herbicides influence nitrate transformation under controlled anoxic conditions representative of nitrate-impacted agricultural subsurface systems. Batch incubations were conducted with 500 µM NO_3^-, either alone or amended with atrazine or desethyl-atrazine, its primary transformation product, each at environmentally relevant trace concentrations (5 µg L^{-1}). Time-resolved quantification of NO_3^-, NO_2^-, NH_4^+, and total dissolved inorganic nitrogen (DIN) enabled rigorous mass-balance evaluation of nitrogen partitioning.

Atrazine enhanced nitrate reduction rates by up to a factor of 45-fold relative to the control and promoted a substantial ammonium accumulation, leading to conservation and retention of dissolved inorganic nitrogen. Desethyl-atrazine accelerated nitrate reduction (~35-fold) but generated a delayed and amplified nitrite peak with contrasting downstream redistribution. Across treatments, nitrate reduction proceeded without measurable DIN loss, demonstrating that accelerated nitrate consumption can coincide with internal nitrogen retention rather than export.

These findings identify nitrite as a dynamic branching node sensitive to subtle molecular differences among co-occurring contaminants. Minor structural variation between parent compound and metabolite redirected electron flow within the nitrogen redox network and modulated whether reduced nitrogen accumulated in dissolved form or followed alternative pathways.

Integrated concentration data and compound-specific isotope measurements ($\delta^{15}N$–$\delta^{18}O$ of NO_3^-/NO_2^- and $\delta^{15}N$ of NH_4^+) were incorporated into a mechanistic reactive model to calibrate and quantify pathway-specific nitrogen fluxes, resolving nitrite partitioning and characterizing nitrogen retention in co-contaminated subsurface systems.