

Unravelling the role of surface complexation in the isotopic fractionation of Fe aerosols

CECILIA G. PECH¹, JEROEN DE JONG², CARMEN CIOTONEA¹, GUILLAUME DHONT¹, NADINE MATTIELLI³ AND PASCAL FLAMENT¹

¹Université du Littoral Côte d'Opale

²Université Libre de Bruxelles

³Université Libre de Bruxelles (ULB)

Presenting Author: cecilia.pech@univ-littoral.fr

Atmospheric deposition is one of the main sources of iron (Fe) in the oceans, where low concentrations of this element affect the global carbon cycle by limiting primary production of marine phytoplankton. While *mineral dust* is often considered the major source of atmospheric Fe, *anthropogenic particles* (mainly pyrogenic) typically display an Fe solubility order of magnitude higher compared to the former ones, which promotes Fe bioavailability. Although Fe isotope signatures ($\delta^{56}\text{Fe}$) have emerged as a sensitive tool for identifying and distinguishing Fe sources to the ocean, traceability of Fe aerosols remains challenging due to the physicochemical processes to which they are subjected during their atmospheric transport.

In order to address changes in Fe solubility and $\delta^{56}\text{Fe}$ derived from atmospheric processing of Fe aerosols, we perform lab-scale experiments using oxalic acid solutions to mimic cloud water, since oxalate is one of the most effective anions in promoting Fe dissolution. As previous studies show that the dissolution under UV/VIS irradiation of both, mineral dust and anthropogenic particles, leads to a faster release of ^{54}Fe [1,2], in this work we focus on determining the influence that the adsorption configuration of oxalate has on Fe isotope fractionation.

Therefore, we present here the results of a combined experimental and theoretical approach that follows the isotopic fractionation of hematite particles in an oxalic acid solution along time. Iron isotopic compositions were determined from batch experiments carried out under light irradiation at different time intervals. Measured values are then compared with theoretical estimations of the fractionation between dissolved and surface Fe-oxalate complexes based on Density Functional Theory (DFT) calculations.

References:

[1] Mulholland, D.S. *et al.* (2021), *Atmos. Environ.* 259, 118505

<https://doi.org/10.1016/j.atmosenv.2021.118505>

[2] Maters, E.C. *et al.* (2022), *Chemosphere* 299, 134472

<https://doi.org/10.1016/j.chemosphere.2022.134472>