

The Research Group

Analytical, Environmental and Geo-Chemistry

has the honor to invite you to the public defense of the PhD thesis of

Jordi Sans-Duñó

to obtain the degree of Doctor of Sciences

Joint PhD with the University of Lleida (UdL)

Title of the PhD thesis:

Measuring the availability of metals in large mixtures with Diffusive Gradients in Thin-films (DGT) devices

Promotors:

Prof. dr. Jaume Puy (UdL)

Prof. dr. Joan Cecilia (UdL)

Prof. dr. Yue Gao (VUB)

The defense will take place on

Tuesday, July 4th, 2023 at 10h in aula de graus, ETSEA (UdL), Lleida, Spain

The defense can also be followed through a live stream:

<https://eu.bbcollab.com/quest/9acb79cc779944909fedfb51d6835654>

Members of the jury

Prof. dr. Francesc Mas (University of Barcelona, chair)

Prof. dr. Carlos Rey (UdL, secretary)

Prof. dr. Frederik Tielens (VUB)

dr. Pablo Lodeiro (UdL)

Em. prof. dr. Willy Baeyens (VUB)

Prof. dr. Sergi Diez (IDAEA-SCIC)

Curriculum vitae

Jordi Sans-Duñó has completed his bachelor's degree in Chemistry and obtained his MSc on computational modelling in Physics, Chemistry and Biology at the University of Barcelona (UB). Afterwards, he was awarded a PhD grant in the University of Lleida (UdL) to study metal availability in large mixtures with DGT devices. During his research stay at AMGC, he became a joint PhD student at VUB where he has analysed Hg availability in presence of DOM and supervised one MSc thesis. During his PhD he has co-authored three articles in international peer reviewed journals, two of them as first author.

Abstract of the PhD research

Trace-metals are a source of nutrients or toxic agents depending on their concentration and speciation. The speciation is the distribution of the total concentration of an element among its possible species. It is a relevant concept to understand the bioavailability of trace-metals to plants or microorganisms, because the uptake depends, in many cases, on the mobility and kinetics of dissociation of the compounds present in the system. To tackle this problem, this PhD thesis has focused on the development of the interpretation of the experimental data of Diffusive Gradients in Thin-films (DGT) to measure metal availability in natural waters.

DGT is a passive sampler that mimics the physicochemical processes involved in the uptake of metals by measuring a flux of metal that receives the surface of microorganisms and algae. The flux is, then, expressed as a free metal concentration that would produce the same accumulation in a system with only free metal. This concentration is known as the available DGT concentration (C_{DGT}).

In this thesis, we have developed a theoretical framework that allows us to split C_{DGT} in terms of the concentration, mobility and lability of each metal species present in the system.

To this end, we produced experimental measurements in laboratory conditions or in natural waters with DGT devices with different geometric configurations (i.e increasing the thickness of the gel, or adding a stack of 2 resins) to have access to complementary information about the system. Simple analytical expressions involving the lability of the complexes lead to obtain intrinsic parameters of the metal complexes such as the diffusion coefficient and the dissociation reaction rate constant. To validate the result of the analytical expressions we perform also numerical simulations that solve the diffusion-reaction equations with the boundary conditions of the DGT technique. This allow us to predict the experimental accumulation under certain conditions of the system.