ABSTRACT BOOK



SETAC Europe 30th Annual Meeting Open Science for Enhanced Global Environmental Protection

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Online Meeting





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ABSTRACT BOOK SETAC Europe 30th Annual Meeting

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This book compiles the abstracts from the platform and poster session presentations at the 30th Annual Meeting of the Society of Environmental Toxicology and Chemistry - Europe (SETAC Europe), conducted as a virtual conference, from 3–7 May 2020.

The abstracts are reproduced as submitted by the author and accepted by the Scientific Committee. They appear in order of abstract code and alphabetical order per presentation type. The poster spotlight abstracts are included in the list of poster abstracts. The presenting author of each abstract is underlined.

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SOCIETY OF ENVIRONMENTAL TOXICOLOGY AND CHEMISTRY

In the 1970s, no forum existed for interdisciplinary communication among environmental scientists, biologists, chemists, toxicologists, managers, engineers or others interested in environmental issues. The Society of Environmental Toxicology and Chemistry (SETAC) was founded in North America in 1979 to fill the void, and quickly saw dynamic growth in the Society's membership, meeting attendance and publications.

A unique strength of SETAC is its commitment to balance the scientific interests of government, academia and business. The Society by-laws mandate equal representation from these three sectors for officers of the World Council and Geographic Unit Boards of Directors and Councils, and in the composition of committees and other society activities. The proportion of members from each of the three sectors has remained nearly equal over the years.

The Society is concerned about global environmental issues. Its members are committed to Environmental Quality Through Science[®], to timely and effective communication of research, and to interactions among professionals so that enhanced knowledge and increased personal exchanges occur. Therefore, SETAC publishes two globally esteemed scientific journals and convenes annual meetings around the world, showcasing cutting-edge science in poster and platform presentations. Because of its multidisciplinary approach, the scope of the science of SETAC is broader in concept and

application than that of many other societies.

SETAC's growth is reflected in the founding of geographic units around the world. SETAC Europe was established in 1989 as an independent organisation, followed by SETAC Asia-Pacific in 1997 and SETAC Latin America in 1999. In 2002, the four existing organisations joined together under the governance of the SETAC World Council. SETAC Africa is the most recent geographic unit, which was adopted in 2012. As evidence of international acceptance of the SETAC model and of the great interest at the local level, regional chapters and branches have emerged in a number of countries.

SETAC publishes two journals: Environmental Toxicology and Chemistry (ET&C) and Integrated Environmental Assessment and Management (IEAM). Environmental Toxicology and Chemistry is dedicated to furthering scientific knowledge and disseminating information on environmental toxicology and chemistry, including the application of these sciences to risk assessment. Integrated Environmental Assessment and Management focuses on the application of science in environmental decision-making, regulation, and management, including aspects of policy and law, and the development of scientifically sound approaches to environmental problem solving. Together, these journals provide a forum for professionals in academia, business, government, and other segments of society involved in the use, protection, and management of the environment for the enhancement of ecological health and human welfare.

SETAC books provide timely in-depth reviews and critical appraisals on scientific subjects relevant to understanding a wide range of contemporary topics pertaining to the environment. These include any aspect of environmental chemistry, toxicology, risk assessment, risk management, or environmental policy.

SETAC has two administrative offices, in Pensacola, Florida, USA, established in 1992, and in Brussels, Belgium, established in 1993.

prospectively or retrospectively use the REACH registration process to identify PMT/vPvM substances. Special considerations for data uncertainty are presented via the implementation of a "traffic light" system. The guidance was applied to all 15469 REACH registered substances as of May 2017. The list of PMT/vPvM substances is provided and discussed in terms of monitoring data, emission likelihood and current restrictions or regulations.

3.17.4

P chemicals and water resources TF: SETAC Dublin 2020 - Abstract submission for poster presentation

S. Pawlowski, BASF SE; L. Aicher, Swiss Centre for Applied Human Toxicology (SCAHT); A. Berends, SOLVAY / HSE; P.K. Curtis-Jackson, Environment Agency (England and Wales) / Chemical Assessment Unit; K. Doornebosch, Nouryon; J. Franklin, Independent Scientist; M. Greener, Syngenta Ltd; J. Hollender, Eawag / Department of Environmental Chemistry; B. Jene, BASF SE / Environmental Fate; K. Jenner, Givaudan / Global Regulatory Affairs & Product Safety; A. Kowalczyk, SC Johnson EurAFNE Limited / Global Safety Assessment & Regulatory Affairs; D. Lewis, Syngenta; A.D. Redman, Exxon Mobil Biomedical Sciences, Inc. / Toxicology and Environmental Research and Consulting; N. Wang, Total; J.R. Wheeler, Shell International; G. Sanders, Givaudan International SA / Regulatory Affairs and Product Safety; A. Häner, F. Hoffmann-La Roche Ltd / Group SHE (LSR); S. Mardsen-Jones, Environment Agency

Chemicals from various sources may be released into the environment and potentially reach ground- and drinking water resources. The PMT/vPvM-concept was developed by the German Environmental Protection Agency (UBA) with the aim to better protect these resources from such substances regulated under REACh. However, the exercise indicated that hazard-based data evaluation resulted in a serious number of false positive and a certain number of false negative candidates which indicates an urgent need for further adjustment of the concept. Furthermore, available monitoring data illustrated a broader range of substances, which are not REACh-related, that are present in ground- and drinking water and these substances will not be addressed by the REACH PMT/vPvMconcept. An ECETOC Task Force was established to elaborate relevant topics central to such an approach. These included a review of existing legislations, elaboration of the applicability of an alternative risk-based approach, review of existing monitoring data and the level of relevant metabolite concentrations, possibility of NER-formation, appropriateness of the chosen Persistence (P) Mobility (M)- and Toxicity (T) criteria. Results: A risk-based approach using available phys.-chem. and e-fate parameters is applicable. A survey of monitoring data revealed no correlation with logKoc. Employing a 0.1% as relevant metabolite threshold is not practically applicable due to expected low concentrations (≤1ng/L). In EU plant protection product (PPP) regulation, metabolite thresholds are 10% and 5%. NERs are not relevant for water-soluble substances. M cannot be a stand-alone criterion to identify substances with leaching potential to ground and drinking water resources. Including the additional T-criteria will not significantly contribute to an enhanced safety of drinking water. Discussion and conclusion: A risk-based approach is a suitable alternative, compared to the initial hazard based PMT/vPvM-concept, as it allows for the exclusion of both false positive and false negative candidates. For this purpose, additional higher tier data may be required on a case by case basis. The results from the monitoring survey suggests that PMT may not be predictive of actual exposures. A 10% and 5% threshold level for metabolites similar to PPP is recommended. The criteria for 'T' as set out in Annex XIII of REACH already fulfils the protection goal of ensuring human and environmental safety in a conservative manner.

Potential Roles for Diffusive Gradient in Thin Film (DGT) Passive Samplers in Investigative and Regulatory Monitoring

3.18.1

Time-weighted average concentrations with Diffusive Gradients in Thin films (DGT)

<u>J. Puy</u>, Universitat de Lleida and AGROTECNIO; A. Altier, Universitat de Lleida and AGROTECNIO / Dep Quimica; J. Cecilia, Universitat de Lleida and AGROTECNIO / Dep Matemàtiques; C. Rey-Castro, Universitat de Lleida and AGROTECNIO / Dep Quimica; J. Galceran, Universitat de Lleida / Dep Quimica Passive sampling can be a cost-effective analytical approach to provide timeweighted average (TWA) concentrations of pollutants in natural waters. DGT differs from other passive samplers basically by incorporating a diffusion disc in between the accumulation element (binding phase) and the sample [1]. This allows measurements independent of the convective phenomena in the sample solution and a simple interpretacion of the accumulation based on Fick's first law. The effective concentration that results from this interpretation is called *c*_{DGT}, which stands for the metal concentration in a system with only metal that would lead to the same accumulation than the natural sample. In terms of the real species, *c*_{DGT} can be understood as the addition of the free metal concentration plus the labile fraction of the rest of metal species, the contribution of each one being dependent on the respective mobilities [2]. By deploying a DGT device in succesive solutions of different concentrations of Ni, Cd or NiNTA, the use of c_{DGT} as a surrogate of the average experimental total metal concentration for different deployment times and metal concentrations is discussed. When the accumulation in simple metal solutions approaches perfect sink conditions, it is shown that c_{DGT} provides a good estimation of the TWA metal concentration. Transient effects following concentration jumps are mainly dependent on the pulse time, but in a set of oscillating concentrations they tend to cancel out due to the opposite effect of the transient on the difference between cDGT and the experimental average concentration. In presence of ligands, cDGT tends to underestimate the average total metal concentration as seen in many cases. For a dominant strong complex and excess of ligand conditions, a simple factor applied to cDGT can improve the estimation of the TWA concentration as seen in NiNTA solutions[3]. [1] Davison et al. Environ. Chem. 9 (2012) 1-13. [2] Altier et al. Environ. Chem. 15 (2018) 183-193 [3] Altier et al. Anal. Chim. Acta, 1060 (2019) 114-124 Acknowledgement - The authors gratefully acknowledge support for this research from the Spanish Ministry MCIU/AEI (Project CTM2016-78798) and FEDER UE

3.18.2

Can the existing Environmental Quality Standards (EQS) be adapted for Diffusive Gradients in Thin films (DGT), for the chemical assessment of transitional and littoral waters? Yes, we can!

M. Belzunce, AZTI Foundation / Marine Research; I. Amouroux, IFREMER / RBE/BE; M. Belzunce, Azti-Tecnalia; P. Bersuder, Cefas; A. Bettoschi, Università degli Studi di Cagliari / Dipartimento di Scienze Mediche e Sanità Pubblica; T. Bolam, Cefas Lowestoft Laboratory; M. Caetano, IPMA I.P.; M.M. Santos, Instituto Superior Técnico Universidade de Lisboa / Centro de Química Estrutural; J. Franco, Azti-Tecnalia; J. Gonzalez, S. Guesdon, IFREMER; J. Larreta, AZTI Foundation / Marine Research Unit; B. Marras, Università degli Studi di Cagliari / Dipartimento di Scienze Mediche e Sanità Pubblica; B. McHugh, Marine Institute Ireland / Marine Chemistry; I. Mentxaka, FUNDACION AZTI / Marine Research; F. Menet, IFREMER; D. Merkel, Scottish Environmental Protection Agency; V. Millán Gabet, Instituto Tecnológico de Canarias; N. Montero, University of Cagliari; M. Nolan, Dublin City University; O. Perceval, ONEMA DAST; F. Regan, DCU Water Institute, Dublin City University / Chemical Sciences; C. Robinson, Marine Scotland Science / National Health and Environmental Effects Research Laboratory; M. Rodrigo Sanz, Instituto Tecnológico de Canarias; M. Schintu, Università degli Studi di Cagliari / Dipartimento di Scienze Mediche e Sanità Pubblica; B. White, DCU Water Institute, Dublin City University / Chemical Sciences EQS (or related concepts) are being used worldwide based upon a plethora of legislations. As an example, the European Water Framework Directive (WFD; 2000/60/EC) establishes that the chemical status of water bodies must be determined by the comparison of the concentrations of priority substances with EQS. Within the WFD, although there are some EQS for biota, most of them are for water. And, specifically, as far as metals are concerned, they must be evaluated in the dissolved fraction. Within the plethora of systems or methodologies for integrated sampling, Diffusive Gradients in Thin films (DGT) are already widely used in investigative monitoring of metals and there is an increasing interest in their use for the environmental assessment of water bodies, within European policies requirements. However, at this time, it is not possible to use DGT to assess chemical status in water bodies within WFD, as it is not an officially established method and there are no regulatory EQS. Thus, in the context of MONITOOL European project, the overall objective is to adapt the already existing EQSs for water to those for DGTs, enabling their use for regulatory monitoring. In 2018, two campaigns were carried out in winter (rainy season) and in summer (dry season); simultaneous deployment of DGTs and high-frequency collection of spot water samples were carried out. The sampling campaigns were performed in four selected sites (transitional and coastal sites) in each of the eight Atlantic and Mediterranean European regions. Metals were analysed in three fractions: dissolved, chemical labile and DGT. From this data, EQS will be established through a transparent and scientific procedure, to ensure that they are at least as protective as EQS laid down for water, and therefore they will be proposed formally for regulatory purposes within the WFD.

3.18.3

Monitoring of pharmaceuticals, pesticides and perfluorinated compounds in wastewater using a hydrogel-based passive sampler (o-DGT)

<u>B. Vrana</u>, Masaryk University, Faculty of Science, RECETOX / RECETOX; P. Fialova, Masaryk University Faculty of Science / RECETOX Research Centre for Toxic Compounds in the Environment; J. Urík, K. Sverclova, Masaryk University, Faculty of Science / RECETOX; S. Kaserzon, University of Queensland / Queensland Alliance for Environmental Health Sciences (QAEHS); K. Grabicova, University of South Bohemia in CB / Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses; H. Svecova, R. Grabic, University of South Bohemia in Ceske Budejovice / Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses Several configurations of passive samplers based on diffusive gradients in thin the absolute concentrations in the groundwater, and relative changes between river and groundwater against log KOC, and other physicochemical properties relative to common reporting thresholds. The chemicals were further benchmarked against available ready biodegradation test data. The analysis indicates the presence of some chemicals in ground water and surface water was not correlated with log Koc or with the biodegradation results. This indicates that log Koc-based M criterion, or even the P screening criteria, are not necessarily predictive of exposures through drinking water. This is likely due to the prevailing importance of exposure scenarios (amount, pathways) over the importance of the intrinsic properties of the substance as well as additional processes and mechanisms acting on the fate of chemical substances under natural environmental conditions.

3.17P.9

Consideration of Relevant Metabolites in the Context of the PMT Concept and Protection of Water Resources

M. Greener, Syngenta Ltd; A.D. Redman, Exxon Mobil Biomedical Sciences, Inc. / Toxicology and Environment Science Division; S. Pawlowski, BASF SE The PMT/vPvM-concept is proposed to be applied to REACh registered substances and its transformation product(s). For metabolites, the relevance threshold was set as 0.1% (w/w) of the parent (similar to PBT assessments). The applicability of this threshold was reviewed in light of the existing data requirements for plant protection products, the OECD 307, 308 and 309 TGs, and, taking into account relevant ECHA/Board of Appeal decisions. Furthermore, the logic behind increased mobility of substances/metabolites and the possibility of non-extractable residue (NER) formation were evaluated. Experience with plant protection products indicates that metabolites are considered as relevant if they are $\geq 10\%$ (w/w) at any time during the study, or any that appeared twice at $\geq 5\%$, or, if the concentration is increasing towards the test end and the metabolite level is ≥5%. The OECD 307, 308 and 309 TGs recommend using environmentally relevant concentrations to derive more realistic biodegradation kinetic data. For industrial chemicals, predicted environmental concentrations (PECs) are typically in the range of 0.01 to 10 μ g/L, which corresponds to a relevant metabolite concentration of 0.01 to 10 ng/L, which is consistent with the prioritisation exercise of the EU Water Framework Directive. An evaluation threshold of 0.1% is analytically very challenging and may not always be possible. The low concentrations result in relatively low risks from metabolites, especially since for industrial chemicals they have a relatively lower contribution to risk than the parent itself. Additionally, the measurement of non-extractable residues (NER) depends on the test conditions and the extraction methods, although the risks from these NERs remains unclear due to limitations in bioavailability. For example, formation of biomass through metabolism should not be part of a persistence assessment. However, the speciation of NER (e.g., bound vs biomass) is difficult to achieve experimentally and difficult to interpret mechanistically due to variable test methods that have undergone limited validation. Due to these uncertainties, the ECETOC recommendations on NER include estimates of bioavailability to quantify their contribution to risk. By their very nature, risks due to NER are lower than the extractable material. To conclude, setting a threshold of 0.1% (w/w) for relevant metabolites, is not applicable to most of the industrial chemicals on the EU market and the relevance of NERs is low.

3.17P.10

Review of predictive risk assessment approaches for the transport of chemicals to groundwater. A proposal for an improved tiered approach for use in Regulation

N. Vallotton, Dow Europe GmbH / Toxicology Environmental Research and Consulting; M. Greener, Syngenta Ltd

The management of drinking water resources aims at providing water in sufficient quantity and quality and, as a consequence this objective is reflected in European regulations (EU Drinking and Ground Water directive). Acknowledging the different sources and release patterns of chemicals in the environment, regulations aiming at the proactive protection of humans and the environment from chemicals, such as the Plant Protection Product Regulation or the REACH Regulation, include groundwater in their assessment frameworks. Several risk assessment tools have been developed to model and predict the leaching of chemicals to groundwater for the purpose of risk assessment in order to proactively protect drinking water. Information typically needed to support the assessment include the substances properties, such as the physical-chemical and fate properties, the characterization of the environmental compartment(s) of release and the associated rates of emissions. Several risk assessment models were reviewed with a focus on routes of exposure addressed, key metrics supporting the exposure assessment and their level of conservatism. Independently of the model, the application rate to soil or dose applied to land is an important driver of the magnitude of exposure. The sensitivity analysis performed with fictional substance with a range of half-lives in soil and partitioning to organic carbon (Koc) provides contrasting results illustrating the important of the route of exposure to soil. For chemicals with direct application to soil, the potential to reach groundwater is greater for substances with a slow degradation in soil and low Koc. In contrast, chemicals released down the drain may have exposure in soil as consequence of sludge application to land, however a prerequisite of such exposure is adsorption to sewage sludge. Substance with slow degradation thus

also have a greater potential for exposure in soil, but the magnitude of such exposure is greater for substance having a high binding affinity to sludge. A tiered risk assessment approach is proposed by the ECETOC task force on "Persistent chemicals and water resources protection" to support an improved screening assessment of potential groundwater contaminant, and as a risk-based alternative to PMT/vPvM criteria.

3.17P.12

Scientific and regulatory challenges to deal with "mobile" substances. A. Jánosi, CEFIC - European Chemical Industry Council; S. Van de Broeck, European Chemical Industry Council - CEFIC / Product Stewerdship Protection of drinking water remains a priority for industry. The recently proposed Persistence, Mobil, and Toxic (PMT) prioritization scheme is being debated as a possible tool to support the maintenance of high quality drinking water. Identification of Mobile and Persistent substances is not a straight forward exercise. Several parameters have to be considered to address the scientific and regulatory complexity. For example, monitoring data, use patterns, and appropriate physicochemical and degradation properties can influence the exposure profile of chemicals in drinking water. Implementation of incomplete prioritization schemes can result in mis-direction of resources with limited, and inefficient impacts on our goals to protect drinking water resources. The presentation will focus on some food for thought on scientific and regulatory challenges encountered to identify these chemicals as well as indication on challenges and potential way forward to address them in the regulatory framework.

3.17P.13

Necessity of Joint Consideration of Persistence and Mobility for Determining the Leaching Risk of Chemicals

B. Jene, BASF SE / Environmental Fate; A. Kowalczyk, SC Johnson EurAFNE Limited / Global Safety Assessment & Regulatory Affairs; P.K. Curtis-Jackson, Environment Agency (England and Wales) / Chemical Assessment Unit; J. Franklin, Independent Scientist; S. Marsden-Jones, wca-consulting In the UBA proposal, P/vP and M/vM are assessed separately. Those chemicals which fulfil the UBA definition of both M/vM and P/vP, are taken into consideration for PMT/vPvM categorisation (with exceedance of the T threshold also being required for attainment of PMT status). This approach produces on the one hand many false positives, substances that are classified PMT/vPvM although they do not reach the groundwater used for drinking water in a considerable amount. On the other hand, it is not excluded that substances are classified false negative and are excluded from further assessments although they may pose a risk to reach groundwater. Despite the need of a combined consideration of soil degradation and sorption, the metrics proposed by UBA may be deemed adequate only for preliminary screening of a large dataset of chemicals, but they present scientific shortcomings that preclude them from being used for any definitive regulatory classification. The main limitations are: • The Koc concept used for the M classification is not valid for soils with low organic carbon content as well as for polar or ionised substances. • Non-consideration of non-linear of sorption. Concentration dependent sorption is mostly observed for chemicals resulting in non-linear isotherms showing increasing sorption with decreasing concentrations. • Non-consideration of slow kinetic sorption also called "aged sorption". This process causing the well-known phenomenon of hysteretic sorption (desorption deviate from adsorption isotherms) is the expression of considerable increase of chemical sorption with time and must not be ignored. • Competitive sorption which is not considered in the Koc concept can lead to displacement of a sorbed species by another. •

Immobilisation through formation of NER Due to the inadequacy seen with the proposed concepts to identify the leaching risk, alternative approaches are discussed: • Leaching indices combining the main chemical characteristics such as degradation and sorption. • Ranking approach as used by the CIS Working Group to setup the Groundwater Watch List. •

Risk assessment approach based on modelling of the leaching potential using models that consider the essential processes and taking into account relevant pedo-climatic scenarios.

Potential Roles for Diffusive Gradient in Thin Film (DGT) Passive Samplers in Investigative and Regulatory Monitoring (P)

3.18P.1

High frequency measurement of metals: steps towards the acceptance of passive samplers for regulatory monitoring

I. Krikech, Abdelmalek Essaâdi University; <u>I. Mentxaka</u>, FUNDACION AZTI / Marine Research; M. Belzunce Segarra, Azti-Tecnalia / Marine Research; J. Franco, Azti-Tecnalia; J. Larreta, AZTI Foundation / Marine Research Unit; J. Rodríguez, AZTI Foundation

Diffusive Gradient in Thin Films (DGT), and passive samplers (PS), in general, are already widely used in investigative monitoring and there is an increasing interest in their use for the environmental assessment of water bodies, within

European policies requirements. In the regulatory context of the European Water Framework Directive (WFD) (2000/60/EC), the main barrier for the acceptance of PS is the lack of appropriate Environmental Quality Standards (EQSs). Regulatory EOSs for metals in water are defined in the dissolved fraction, preventing the use of DGT-labile concentrations for the establishment of the chemical status of water bodies. The specific objectives of this study are: to investigate the relationship between dissolved metal concentrations from spot sampling with DGT-labile metal concentrations, to evaluate the reliability of the techniques for the measurement of metal concentrations in estuaries and to provide recommendations for the use of DGTs to develop environmental guidelines. In November 2019, five samplings were carried out in the Oiartzun estuary (Basque Country, Bay of Biscay), an area with high presence of industrial and port activities. DGTs (triplicates) were deployed and retrieved after 12 hours. During that period, hourly spot water samples were taken, at the same depth than DGTs. Water samples were filtered for the posterior analysis of metals, dissolved organic carbon and the quantification of suspended particulate matter (SPM). Priority metals (Cd, Ni, Pb) and other specific metals (Al, Ag, Cu, Cr, Co, Fe, Mn, Zn) were analysed in the 2 defined fractions (dissolved and DGT fraction) by ICP-MS. Hydrographic variables were measured at each sampling time. The relationships between dissolved and labile metal concentrations and the environmental factors influencing such correlations were studied. The results show that dissolved Ni and Cd can appear mostly labile and available for uptake by DGTs, while most of the dissolved Cu, Pb and Zn can be forming organic complexes no detected by DGTs. Statistical analysis highlighted the relationships between metal concentrations in DGT and in spot water samples, together with the variability in relation to the hydrographic variables. Acknowledgement - Monitool project (https://www.monitoolproject.eu) (nº contract: EAPA_565/2016) is co-financed by the European Regional Development Fund through the Interreg Atlantic Area Programme and by the Basque Water Agency.

3.18P.2

Impact of temperature, seasonality and metal concentration on DGT membrane biofouling in marine envrionments

M. Nolan, Dublin City University; F. Regan, <u>B. White</u>, DCU Water Institute, Dublin City University / Chemical Sciences

Heavy metals as environmental contaminants are of particular concern due to their toxic effects when accumulated within organisms. Under Directive 2013/39/EU, cadmium, nickel, and lead were identified as priority metals of ecological concern in the field of water policy. At present, Environmental Quality Standards (EQS) for these metals only include biota sampling, and therefore the development of new in situ solution sampling methods are a priority. Passive sampling devices (PSDs) allow for the accumulation of an analyte over time, providing a time-weighted average of concentration of the analyte. Their low cost and ease of use offers benefits over traditional point grab sampling or biota sampling. For heavy metals in solution, the most prominent PSD is the Diffusive Gradient in Thin Film (DGT) device. DGT devices are composed of an ionexchange resin, separated from solution by a diffusive ion-permeable gel layer. DGTs measure a labile metal fraction, often considered a bioavailable fraction. In this research, multiple factors were examined to determine their impact on the application of DGT passive sampling devices in a marine environment. Biofouling on DGT devices deployed in marine waters along the Atlantic coast was examined, studying speciation and extent of fouling, particularly in relation to temperature induced effects, and an examination of potential methods to mitigate fouling through the use of alternative membrane filters. Results will be presented here with explore multiple strategies for biofouling impacts to be minimised during DGT deployment.

3.18P.3

Unravelling dynamic characteristics of metal species in mixtures from Diffusive Gradients in Thin films (DGT) measurements

J. Sans-Duñó, A. Altier, Universitat de Lleida and AGROTECNIO / Dep Quimica; J. Cecilia, Universitat de Lleida and AGROTECNIO / Dep Matemàtiques; C. Rey-Castro, Universitat de Lleida and AGROTECNIO / Dep Quimica; J. Galceran, Universitat de Lleida / Dep Quimica; <u>J. Puy</u>, Universitat de Lleida and AGROTECNIO

Dynamic speciation is an important issue to understand and to prevent toxic effects in natural systems. When Diffusive Gradients in Thin films devices (DGT) are used to measure metal availability, all metal species can contribute to the accumulation depending on the respective diffusivities and labilities. Although many efforts have been devoted to the study of simple systems with only one ligand (single ligand system, SLS)[1], the influence of the system composition on the lability of the species is largely unknown. Thus, a series of experiments with DGT (Diffusion Gradients in Thin films) devices [2] were carried out to measure nickel (Ni) accumulations in laboratory solutions containing either Nitrilotriacetic acid (NTA), Ethylenediamine (EN) or mixtures of both ligands. It is shown that NiEN and NiNTA can become more labile and inert (respectively) in the mixture than in the corresponding SLS. As variations in the lability degrees of NiNTA and NiEN arising in the mixture tend to cancel out, the summation of partial fluxes calculated from lability degrees obtained in SLS yields a reasonable estimate of the DGT performance in the mixture [3]. These results pave the way to obtain

dynamic characteristics of mixtures from DGT devices with different thickness of the resin or of the diffusive disc[4]. References: 1 Uribe, R.; Mongin, S.; Puy, J.; Cecilia, J.; Galceran, J.; Zhang, H.; Davison, W. Contribution of partially labile complexes to the DGT metal flux. Environ. Sci. Technol. 45 (2011) 5317-5322. 2 Interpreting the DGT measurement: speciation and dynamics. In Diffusive Gradients in Thin-Films for environmental measurements, Davison, W., Ed.; Cambridge University Press: Cambridge, 2016. 3. Altier, A.; Jimenez-Piedrahita, M.; Uribe, R.; Rey-Castro, C.; Cecilia, J.; Galceran, J.; Puy, J. Effects of a mixture of ligands on metal accumulation in diffusive gradients in thin films (DGT). Environ. Chem. 15 (2018) 183-193. 4. Baeyens, W.; Gao, Y.; Davison, W.; Galceran, J.; Leermakers, M.; Puy, J.; Superville, P.; Beguery, L In situ measurements of micronutrient dynamics in open seawater show that complex dissociation rates may limit diatom growth. Scientific Reports, 8 (2018) 16125 The authors gratefully acknowledge financial support from the Spanish Ministry MINECO (Project CTM2016-78798).

3.18P.4

A New Polar Organic Chemical Integrative Sampler (POCIS) for Linear Alkylbenzene Sulfonate (LAS)

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This study aimed to use the Polar Organic Chemical Integrative Sampler (POCIS) under non-steady-state conditions resulting from natural disasters and environmental accidents. In such conditions, it is expected that a chemical which is stored in large amounts will leak to the aquatic environment easily, and its concentration in the aquatic environment will increase. Therefore, the priority to be prepared should not be decided only for the chemical's toxicity but also the stored amounts.Linear Alkylbenzene Sulfonates (LAS) were widely used as a kind of an anionic surface-active agent in the world. Products including the LAS have been used as household detergents such as laundry powders, laundry liquids, and all-purpose cleaners. However, the LAS are extremely toxic to fishes and water fleas and has been detected in the aquatic environment. In addition, the amount of the LAS stored for industrial use is expected to be huge. For example, the largest stored amount of the LAS in an industry in Osaka, Japan is about 320 tons. Therefore, the LAS were selected as the target chemicals in this study. The peak concentration and a half-life of the LAS in a river contaminated by chemical leak from an industry were estimated by a model. The POCIS is one of the most widely used passive sampler for aquatic environment. Compared to grab sampling, passive sampling has an advantage to measure time weighted average of the target concentration. In short, the passive sampling can measure a short time peak which would be slipped over by the grab sampling. The POCIS which is a strong tool for monitoring hydrophilic organic matter; $0 \leq \log P_{ow} \leq 5$; has been applied for pesticides, pharmaceuticals, perfluorinated compounds, munitions, and drugs. Thus, the POCIS should be suitable for the monitoring of LAS which its $\log P_{ow}$ is 3.32 (calculated as C_{11.6}). We developed a POCIS optimized for the LAS via batch experiments and recovery experiments. Oasis WAX, a mix-mode, Weak AnioneXchange, reversed-phase, water-wettable polymer was chosen as the best receiving phase for the new POCIS from eleven adsorbent candidates including polymer type adsorbents and active carbon type adsorbents. The developed POCIS was validated in a chamber which replicated the non-steady-state condition following to the model results. The results of the chamber experiment indicated that the POCIS was a good tool to be used in emergency.

3.18P.5

Experimental calibration of the copolymer ethylene vinyl acetate (EVA) passive sampler for emerging contaminants in freshwater.

H. Rosales, Universidad de concepcion / Facultad de Ciencias Ambientales y Centro Eula-Chile; F. Tucca, Universidad Andrés Bello / Department of Ecology and Biodiversity; A. Baeza, Universidad de Concepción, Faculty of Environmental Sciences and EULA-Chile Centre, / Environmental Engineering; R.O. Barra, Universidad de concepcion / Aquatic systems Monitoring and quantification of emerging contaminants in freshwater needs the development of new methodological approaches for a detection improvement and in a cost-effective way. Currently, there are various methods of monitoring the occurrence of pollutants such as grab, continuous, automatic and passive sampling. In recent years, the effectiveness of contaminant monitoring has been observed through the use of passive sampling. These devices allow combining the sampling, selectivity and pre-concentration of chemical substances in a single step, using a minimum quantity of solvents in the whole process of extraction and deployment in the field. In this work we present an experimental calibration of the copolymer ethylene vinyl acetate sampler (EVA) by using a calibration system designed in the laboratory. Here, 5 chemicals, with a wide range of Log Kow (from 0 to 5) were considered for the experimental calibration (namely, caffeine, chloridazon, atrazine, ibuprofen and triclosan). The partitioning coefficient between EVA and water (Keva-w) and the sampling rates (Rs) were determined under the experimental flow rate (range 0.05 to 0.25 m/s) and temperature conditions (range 8 to 14 °C). The chemical analyses were conducted both in water and the EVA sampler by HPLC-DAD. The results show that EVA sampler had a good selectivity and adsorption for all chemicals, including the less