TreatRec ITN: Interdisciplinary concepts for municipal wastewater treatment and resource recovery

Message of TreatRec

We test technological aspects and cost-effectiveness of advanced wastewater treatments. Also, we aim to identify the role of treatment units in wastewater treatment plants (WWTP). In both cases the focus is on nutrient recovery and emerging contaminants, but also on energy consumption and reliability of plants.

We research the fate and behavior of under-studied emerging micro-contaminants in waste-water treatment (*Read the introduction below for more info!*).

We check the resilience and robustness of treatments against changes of environment for both the present day and the future. And we support controllers with a decision support system built up with the process knowledge of TreatRec.

Meet us and our projects

Luca Sbardella
Innovative technologies for micro-contaminant removal and resource recovery.

Yaroslav Verkh
Transformation of micro-contaminants in wastewater treatment.

Sara Johannson
Optimal confi-guration of nitrogen and phosphorous recovery in waste-water treatment.

Pau Juan
Resilience of waste-water treatment to multiple stress conditions.

Pau Gimeno
Assessment of environmental and socio-economical implications of urban wastewater system upgrades.

Our workplaces in both business and academia

Atkins Global (UK) is one of the world's leading engineering and design consultancies. It supports the water-related environmental sectors with strategy planning, flood management, infrastructure design and maintenance.

Aquafin is the wastewater treat-ment agency of the Flemish region of Belgium. It handles the design, the financing and the operation of collector sewers and sewage treat-ment plants of an area covering about 13,500 km^2 and 6 million people equivalents.

The Catalan Institute for Water Research (ICRA) in Girona, ES is a research centre which innovates the sustainable use of water. It unites several areas of water research as chemistry, ecology, water technology, and microbiology.

The Laboratory of Chemical and Environmental Engineering (LEQUIA) is a research group at the University of Girona (UdG). It develops eco-innovative water solutions.

Non-targeted analysis of dissolved organic matter in wastewater treatment

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Introduction

Dissolved organic matter (DOM) in wastewater is a mixture of polysaccharides, proteins, lipids, nucleic acids, soluble microbial products and human-made organic chemicals.[1] The human-made chemicals here-in include surfactants, personal care products, phar-maceuticals, pesticides, but also transformation pro-ducts (TP) which appear in course of the treatment. These can be hazardous even at small concen-trations.[2]

Normally the analysis of hazardous substances in DOM limits the scope to a narrow range of hand-picked compounds. It neglects hundreds of chemicals from influent wastewater and those that emerged du-ring treatment. Measurements as of the chemical oxy-gen demand (COD) represent the efficiency of DOM removal at WWTP. Yet the mentioned tools need a lot of expert knowledge to build one data stream.[3]

Analysis of a larger fraction of DOM in wastewater using computational analysis of liquid chromatogra-phy-high resolution mass spectrometry (LC-HRMS) data offers a better understanding of treatments and fate of chemicals therein.[4] The statistical HRMS data analysis started in petroleomics and natural water research. It considers the entire available data, typically 10^3 – 10^5 unknown signals, obtained by LC-HRMS.[5,6] Herein it fingerprints the heterogenic mixture of DOM before and after nanofiltration (NF) and secondary biological wastewater treatments (BT).

Materials and Methods

Feed (influent) and permeate (effluent) grab samples of NF treatment were taken from a pilot WWTP in Quart, Spain. The grab samples of a secondary BT were taken from a municipal WWTP in Celrà, Spain. Then the samples were purified and pre-concentrated through solid phase extraction (SPE).

An LTQ-Orbitrap mass spectrometer coupled with the Aria TLX-1 HPLC system recorded LC-HRMS spectra. The chromatographic separation was achieved on Acquity UPLC® HSS T_3 in the positive electrospray ionization mode (PI) and on Acquity UPLC® BEH C_{18} chromatographic column in the negative ionization mode (NI).

Mzmine 2.23 and an own *R* package extracted the data. The mass tolerance for the processing of LC-MS spectra was 3 ppm. The heuristic rules applied for formula prediction corresponded to those for 99.7% of registered small molecules.

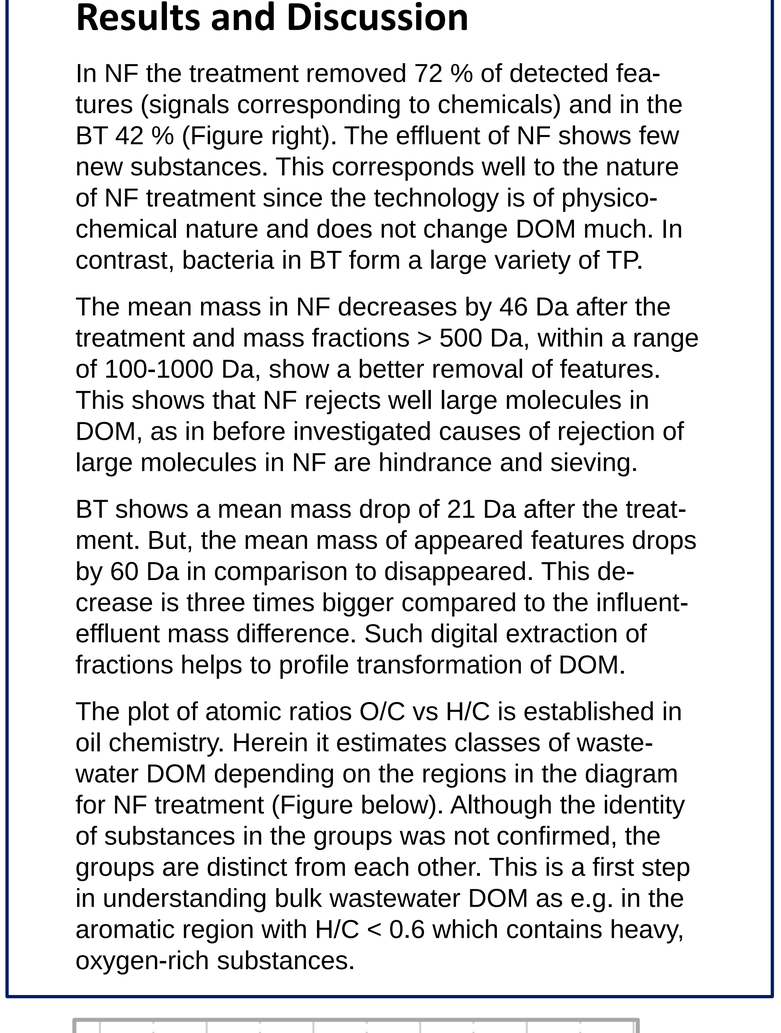
Results and Discussion

In NF the treatment removed 72 % of detected fea-tures (signals corresponding to chemicals) and in the BT 42 % (Figure right). The effluent of NF shows few new substances. This corresponds well to the nature of NF treatment since the technology is of physico-chemical nature and does not change DOM much. In contrast, bacteria in BT form a large variety of TP.

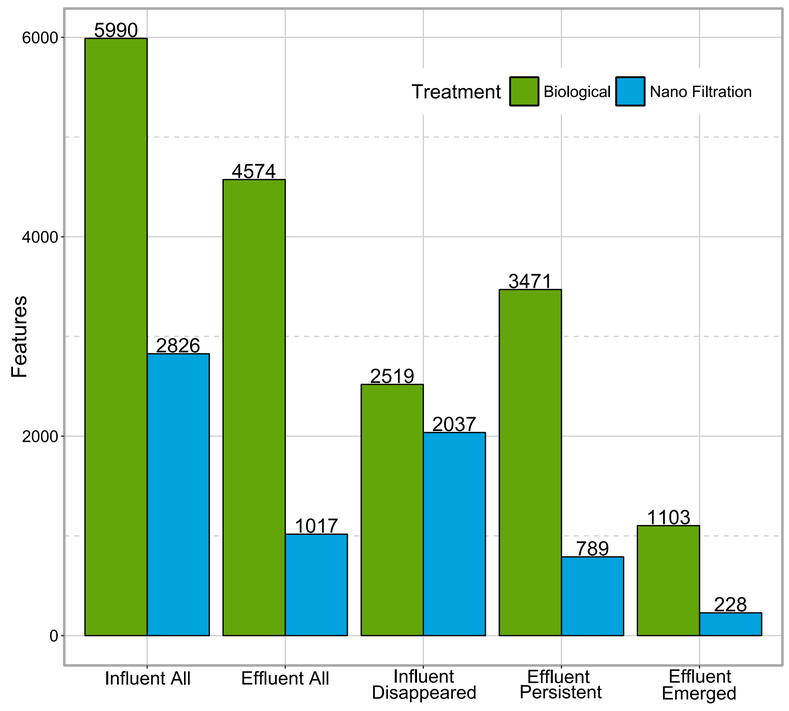
The mean mass in NF decreases by 46 Da after the treatment and mass fractions > 500 Da, within a range of 100-1000 Da, show a better removal of features. This shows that NF rejects well large molecules in DOM, as in before investigated causes of rejection of large molecules in NF are hindrance and sieving.

BT shows a mean mass drop of 21 Da after the treat-ment. But, the mean mass of appeared features drops by 60 Da in comparison to disappeared. This de-crease is three times bigger compared to the influent-effluent mass difference. Such digital extraction of fractions helps to profile transformation of DOM.

The plot of atomic ratios O/C vs H/C is established in oil chemistry. Herein it estimates classes of waste-water DOM depending on the regions in the diagram for NF treatment (Figure below). Although the identity of substances in the groups was not confirmed, the groups are distinct from each other. This is a first step in understanding bulk wastewater DOM as e.g. in the aromatic region with H/C < 0.6 which contains heavy, oxygen-rich substances.



Distribution of atomic ratios for the 2126 features of the influent NF DOM with assigned elemental formulas.



Number of detected LCMS features for either treatment.

Literature cited

(1) Michael-Kordatou, I.; Michael, C.; Duan, X.; He, X.; Dionysiou, D. D.; Mills, M. A.; Fatta-Kassinos, D. *Water Res.* **2015**, *77*, 213–248.
(2) Daughton, C. G. *Environ. Impact Assess. Rev.* **2004**, *24* (7–8), 711–732.
(3) Prasse, C.; Stalter, D.; Schulte-Oehlmann, U.; Oehlmann, J.; Ternes, T. A. *Water Res.* **2015**, *87*, 237–270.
(4) Nürenberg, G.; Schulz, M.; Kunkel, U.; Ternes, T. A. *J. Chromatogr. A* **2015**, *1426*, 77–90.
(5) Hughey, C. A.; Hendrickson, C. L.; Rodgers, R. P.; Marshall, A. G.; Qian, K. *Anal. Chem.* **2001**, *73* (19), 4676–4681.
(6) Remucal, C. K.; Cory, R. M.; Sander, M.; McNeill, K. *Environ. Sci. Technol.* **2012**, *46* (17), 9350–9359.

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