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Editorial

From Detection to Remediation: Analytical Science at the Forefront of Environmental Research

Cite This: *ACS Omega* 2022, 7, 38105−38108

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Analytical science plays a vital role in many aspects of science, but its role in environmental research is perhaps more apparent now than ever before, particularly given the well-publicized and ever-increasing challenges we face from climate change and environmental pollution. The phrase "From Detection to Remediation", used as the title of this editorial, captures how analytical science is a key component in environmental research, in not only the detection and quantification of substances but also extraction and separation of contaminants and the purification and reuse of natural resources for improved environmental health and a more sustainable future.

To showcase the important and multifaceted contributions of analytical chemistry to environmental research, the editors of *ACS Omega*, *Analytical Chemistry*, and *Environmental Science & Technology* (*ES&T*) have each selected recently published works that they consider have advanced these critical applications of analytical science, highlighted here as part of this special virtual issue. This editorial introduces these selected articles that have contributed toward tackling global environmental health issues. It is our belief that the global nature of the challenge of environmental health is reflected in this virtual issue by the geographic and topic diversity of the articles featured in this collection.

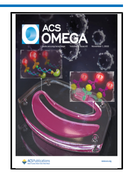
DETECTION AND QUANTIFICATION OF CONTAMINANTS AND POLLUTANTS

A fundamental aspect of analytical science involves precise and accurate measurements. The complexity, cost, and safety of generating an accurate assessment of what is present in different, sometimes complex matrices, and in what quantity is a significant challenge, particularly when the contaminants present are unknown or in complex mixtures. The effective monitoring of air, water, and soil quality has major implications on many aspects of life, including, most immediately, the air we breathe, the water we drink, and the soil we use to grow food and sustain life. All three contributing journals regularly publish recent advances in analytical techniques and approaches toward this aim.

Poor air quality is among one of the leading environmental health concerns. Repeated exposure to pollutants can significantly impact both life expectancy and quality of life. The detection and quantification of pollutant levels in indoor and outdoor environments is an important area of research, as are investigations into the impact of air pollutants on our health. Examples of air quality analysis featured in this virtual issue provide an insightful view of the diversity and complexity of air quality research, from assessing the toxicity and oxidative stress of fine particulate matter in the more heavily industrialized areas of China in an *ES&T* article by Jin et al. (DOI: 10.1021/acs.est.9b00449) to studying the airborne release of microtoxins from inland lake water in the United States in an *ES&T* article by Olsen et al. (DOI: 10.1021/acs.est.9b07727). The detection and quantification of known toxic and flammable gases is of importance for domestic and industrial environments as well as ecological protection. In a mini-review published in *ACS Omega*, Alzate-Carvajal and Luican-Meyer (DOI: 10.1021/acsomega.0c02861) assess recent advances in the preparation and characterization of functionalized graphene and reduced graphene oxide gas sensors to improve selectivity in sensor performance. Gas sensors based on two-dimensional materials also face difficulties with calibration, neatly addressed by Ricciardella et al. (DOI: 10.1021/acsomega.9b04325) with a new method to overcome the lack of steady-state signals during gas exposure and facilitate reliable calibration.

The analysis of water quality is a key aspect of environmental protection. A significant focus of environmental monitoring has been the detection, quantification, and fate of contaminants in varied water sources, as summarized in the article in *Analytical Chemistry* by Richardson et al. (DOI: 10.1021/acs.analchem.1c04640). The detection and monitoring of heavy metals in industrial wastewater has been approached via technologies such as wireless microfluidics (DOI: 10.1021/acsomega.1c00941) and luminescence spectroscopy (DOI: 10.1021/acsomega.0c00270). Surface-enhanced Raman scattering (SERS) is used to sense transition metal ions in water, concisely reviewed by Guerrini and Alvarez-Puebla (DOI: 10.1021/acsomega.0c05261). Pham et al. demonstrated the colorimetric detection of cadmium ions by chelating them in aqueous solution with a polydiacetylene-based sensor, overcoming the cost issue with traditional analytical methods for cadmium ion detection and the selectivity issues often encountered by sensors (DOI: 10.1021/acsomega.0c04636). Xu et al. (DOI: 10.1021/acs.analchem.0c01710) developed aptamer-based sensors for

Published: October 19, 2022



real-time detection of cadmium, and in another novel approach, Zhang et al. (DOI: 10.1021/acs.analchem.9b05508) achieved highly sensitive detection of mercury by developing an amplification technique that integrated quantum dots and liposome carriers.

Another good example of heavy metal monitoring in environmental water samples was published in *ACS Omega* by Matsueda et al. (DOI: 10.1021/acsomega.1c02756). They demonstrated an online solid-phase extraction−inductively coupled plasma−mass spectrometry (ICP-MS) method to quantify ppb levels of technicium-99, a commonly found isotope in marine environments as a result of discharge from nuclear fuel reprocessing plants, in a range of real water samples. One particularly noteworthy aspect of this work is that the automated nature of the sampling and analysis completely circumvents the need for human handling, which is a huge advantage from a safety standpoint when dealing with radioactive material, while serving a vital purpose of monitoring the presence of such material in water supplies. When combined with liquid chromatography, ICP-MS enabled speciation analysis of Ag_2S and ZnS nanoparticles in environmental water samples (DOI: 10.1021/acs.analchem.0c00262).

For organic pollutants such as cyanide, Padghan et al. developed a chemodosimeter-based method for ultrasensitive and selective detection of cyanide across a wide pH range in environmental water samples (DOI: 10.1021/acsomega.0c05409). Bai et al. utilized a colorimetric chemosensor for the quantitative detection of the cyanide anion in aqueous solution assisted by a smartphone app (DOI: 10.1021/acsomega.0c00021). An example of the use of SERS for the detection of organic dyes in liquid medium was demonstrated by Yu et al. in their recent *Analytical Chemistry* article (DOI: 10.1021/acs.analchem.0c03375). Other organic contaminants commonly found in groundwater include hormones and pharmaceuticals, and a recent article from Bexfield et al. details a systematic assessment of the vulnerability of drinking water across the United States to contamination by these compounds (DOI: 10.1021/acs.est.8b05592). The principal finding from the work was the limited extent of contamination of groundwater used for drinking water by these compounds in the United States and that these compounds are unlikely to have adverse effects on human health at the detected concentrations. Another demonstration of the use of smartphone technology in sensing applications was reported in *ACS Omega* by Mukherjee et al. (DOI: 10.1021/acsomega.0c03465). In this article, the authors present a cost-effective, portable device for highly selective and sensitive colorimetric detection and quantification of fluoride anions in groundwater, an important environmental and public health concern because of the health issues associated with overexposure to fluoride.[3,4] Likewise, complementary techniques have been developed for the detection and characterization of per- and polyfluoroalkyl substances (PFAS) in environmental water samples. Dodds et al. (DOI: 10.1021/acs.analchem.9b05364) used liquid chromatography and ion mobility mass spectrometry to characterize PFAS in wastewater. McCord et al. utilized high-resolution mass spectrometry for nontargeted screening and identification of PFAS in the Cape Fear River, North Carolina (DOI: 10.1021/acs.est.8b06017). Recent articles in *Analytical Chemistry* provide neat examples of improving extraction and analysis of PFAS in water. Suwannakot et al. (DOI: 10.1021/acs.analchem.9b05524) used metal−organic frameworks to enhance solid-phase microextraction of perfluorooctanoic acid from tap water, rainwater, and seawater prior to mass spectrometry analysis, while Grandy et al. (DOI: 10.1021/acs.analchem.0c01490) equipped a solid-phase microextraction sampler on a drone, which facilitated surface water sampling from dangerous or difficult-to-reach sites.

Of significant concern in environmental water analysis is the identification, quantification, and characterization of disinfection byproducts formed during the treatment of water for drinking water purposes. Their formation and potential cyto- and genotoxicity make them an increasing concern, especially at a time when wastewater reuse for a sustainable water supply is an increasing reality. In a recent *ES&T* article (DOI: 10.1021/acs.est.0c06109), Qiu et al. demonstrate a nontarget approach to identify and quantify a naturally occurring N-heterocyclic compound in source water that can act as a precursor to several nitrosamines during disinfection treatment, where nitrosamines are probable human carcinogens. The additive effects of multiple disinfection byproducts (DOI: 10.1021/acs.est.0c00958) and suspected drivers of cytotoxicity (DOI: 10.1021/acs.est.1c07998) highlight the need to study the mixtures of DBPs for understanding human health effects and challenges in drinking water quality regulation.

Wastewater epidemiology is a rapidly evolving use of analytical approaches to monitor human population exposures. In their mini-review (DOI: 10.1021/acsomega.1c04362), Picó and Barceló highlighted recent wastewater-based epidemiology advances utilizing mass spectrometry to create a "fingerprint" of the health hazards, habits, and lifestyle of a city's population. Such studies have been conducted previously for estimation of community-level habits such as smoking, illicit substance abuse, and alcohol use,[2] but its recent application for virus surveillance during the ongoing pandemic has gained considerable interest and complemented community-level clinical diagnosis of COVID-19. Feng et al. (DOI: 10.1021/acs.analchem.0c02060) summarized challenges and research needs for molecular diagnosis, emphasizing sampling, detection of viral RNA and proteins, and characterization of antibodies produced in response to infection and vaccination.

The detection, quantification, and characterization of contaminants in soil and sediment address other key environmental matrices, directly impacting agricultural production, food safety, and environmental health and sustainability. In their recent *Analytical Chemistry* article, Zhu et al. developed nanozyme sensor arrays to detect a range of pesticides in soil samples (DOI: 10.1021/acs.analchem.9b05110). Li and co-workers developed a highly sensitive immunoassay to detect trace levels of the flame-retardant tetrabromobisphenol in sediments. Although this chemical is now restricted for new uses in many countries, its widespread continuing use in older products and accumulation in the environment is of concern because of its persistence (DOI: 10.1021/acs.analchem.0c01908).

Analytical science also plays an important role in the discovery, quantification, and characterization of new contaminants of emerging concern (CEC). A recent study by Belova et al. utilized ion mobility−high-resolution mass spectrometry to build a comprehensive database designed to enhance identification of hitherto unknown contaminants and their metabolites in both environmental and human matrices. They also demonstrated its applicability to screen for "unknowns" present in human urine samples (DOI:

https://doi.org/10.1021/acsomega.2c06631
ACS Omega 2022, 7, 38105−38108

10.1021/acs.analchem.1c00142). Tian et al. reported the use of mass spectrometry for characterizing CECs through nontargeted and suspect screening of urban marine water (DOI: 10.1021/acs.est.9b06126). Micro- and nanoplastics present another need for improved analytical methods. The persistence and accumulation of plastic fragments in the environment due to low degradation rates is a serious environmental issue because of the potential harm they can cause to ecosystems and human health. A range of promising analytical techniques have recently emerged to enable characterization and quantification. Livermore at al. (DOI: 10.1021/acs.analchem.9b05445) utilized Raman spectral imaging and chemometric analysis to detect and identify airborne microplastics, while Munno et al. developed an application-based library of Raman spectroscopy parameters to identify microplastics, supplemented with information on color, morphology, and size, based on representative samples found in the environment (DOI: 10.1021/acs.analchem.9b03626). An automated analytical method combining FTIR hyperspectral imaging and machine learning has also recently been applied to identify and quantify these materials (DOI: 10.1021/acs.analchem.0c01324). As well as assessing the impact of micro- and nanoplastics themselves, work is also ongoing to understand microbiome interactions with different types of plastics, a good example of which was recently published in *ES&T* by Bhagwat et al. (DOI: 10.1021/acs.est.0c07952). This study investigated the interactions between plastic and marine biofilm-forming microorganisms incubated in a marine environment using a whole-genome sequencing approach. Micro- and nanoplastics are of concern, but also they contain and transport mixtures of plastic-derived chemicals. In an *ES&T* article, Zimmerman et al. (DOI: 10.1021/acs.est.9b02293) benchmarked a range of plastic polymer types for their chemical and toxicological signatures using bioassays and nontarget mass spectrometry.

PURIFICATION AND RECYCLING OF RESOURCES

The identification, detection, quantification, and characterization of pollutants in environmental matrices provide the opportunity to act on this information and provide opportunities for remediation. This also presents a range of technical, practical, and economic challenges, especially given the pressing need to achieve this feat through sustainable means. As such, the efficient extraction or separation of pollutants and the purification of crucial resources such as air, water, and soil remain highly fertile areas of research for analytical scientists who have produced a plethora of promising technologies. Highlighted here are just some examples of the high-quality and impactful work in these areas.

In their recent *ACS Omega* article, Budnyak et al. addressed the important issue of recycling cobalt(II), a key component in lithium ion batteries, using a kraft lignin−silica composite as a highly effective sorbent in aqueous solutions (DOI: 10.1021/acsomega.0c00492). Critically, the sorbent was shown to be recoverable and reusable, was produced from a sustainable source, and not only showed potential for improving the supply and environmental concerns surrounding the use of cobalt in materials such as batteries but also provided insight toward better methods to recycle battery components and to recover a valuable resource.

Much work has been conducted in recent years to mitigate water eutrophication caused by excessive release of nutrients into water bodies, for example, by phosphorus contamination of freshwater supplies. Koh et al. (DOI: 10.1021/acsomega.9b03573) present an elegant solution using a lanthanum-modified polyacrylonitrile membrane for the removal of phosphates from water. The work not only shows promise as an ultrafiltration membrane but also fulfills sustainability goals of low-cost materials and low-energy consumption.

The emergence of micro- and nanoplastics as a serious long-term environmental pollutant has necessitated the development of methods to isolate and remove these contaminants from environmental matrices. Methods such as membrane filtration followed by cloud point extraction (DOI: 10.1021/acs.analchem.0c04996) and field-flow fractionation coupled with Raman spectroscopy (DOI: 10.1021/acs.analchem.9b05336) are among the exciting developments recently published in this area.

CLOSING REMARKS AND FUTURE OUTLOOK

As showcased in this virtual issue, analytical science plays a fundamental role in advancing our understanding of environmental contamination issues, identifying protection goals, and enabling remediation and reuse strategies. As we strive to improve current technologies and develop new ones, trends are appearing in the increasing use of hand-held and remote-use technologies and machine-learning techniques for large monitoring data sets and their interpretation in real-time. As is true across many areas of science, we also observe an increased emphasis on both the cost-effectiveness and sustainability of the solutions that analytical scientists provide to investigate ongoing human and ecosystem health challenges, and we foresee that these will be key considerations that drive future research and dictate which technologies see real-world use.

It is also clear that many technical and practical challenges remain and that facilitating further progress toward a healthier and more sustainable environment will require contributions from all disciplines of science. Through the innovation and creativity of ACS journal authors, we look forward to seeing this field continue to grow, and we eagerly anticipate receiving the fruits of researchers' labor at our journals in the future.

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Notes

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ACKNOWLEDGMENTS

The authors would like to acknowledge the sad passing of Prof. María C. Moreno-Bondi and to place on record our appreciation of her contributions both to this Virtual Issue and to *ACS Omega* as a valued Editorial Advisory Board member.

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https://doi.org/10.1021/acsomega.2c06631
ACS Omega 2022, 7, 38105−38108