Knowns and unknowns of novel entities

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Voices

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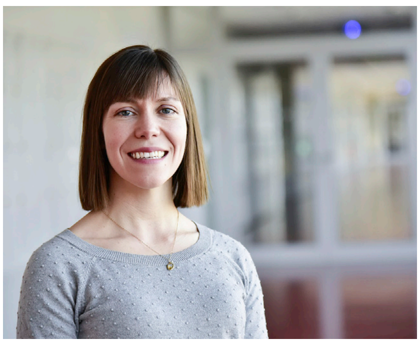
New synthetic chemicals and materials are rising rapidly and are already widespread as novel entities in our daily lives. Although knowledge of their disruptive and long-lasting effects on the Earth system is accumulating, unknowns remain. This Voices asks: what risks do novel entities pose, and what are the emerging concerns?



Lisa Melymuk
RECETOX, Masaryk University

Reduce novel entities through chemical simplification

Historically, pollution has been visible: industrialization, urbanization, and 20th-century farming techniques led to sulfurous smogs, traffic pollution, eutrophic waters, and even burning rivers. Today, novel entities bring a different challenge; their environmental presence is not easily visible, and their health impacts are chronic and subtle. The harm of these "invisible" and largely unknown substances is potentially vast, yet current scientific and regulatory strategies touch only the tip of the chemical iceberg of novel entities.

To deal with this chemical iceberg we rely on high-throughput screenings, advanced instrumental techniques, chemical grouping, read-across, and other strategies to increase the number of substances for which we have a reasonable understanding of chemistry, environmental fate and transport, and toxicity. Yet the challenge is growing; the number of chemicals in commerce is rapidly increasing, disconnected from a complete understanding of their environmental and biological interactions. We cannot solve this problem only by improving our ability to characterize novel entities—chemical simplification must be a part of the strategy. It is an approach to reducing the number of chemicals used in products and adopting smart systemic assessments to more efficiently and accurately analyze chemical risks for the same chemical class. The EU Chemical Strategy for Sustainability (essential use, safe and sustainable by design) touches on some aspects, but a comprehensive effort combining chemical simplification with a true implementation of the precautionary principle is needed to address the challenge of the knowns and unknowns of novel entities.

Laura Carter
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Reuse of waste in agriculture: What are the risks?

In the context of increasing food demand, climate change and the drive toward a circular economy, the reuse of "waste" resources (e.g., wastewater, sludges, and animal manures) to meet irrigation and crop nutrient requirements offers a means of sustainably improving agricultural productivity. However, the use of these "waste" resources inadvertently introduces a suite of chemical pollutants into our soils. While permissible thresholds have been set for more well-studied chemicals such as heavy metals, the same evidence base upon which this regulation is built does not exist for emerging contaminants such as human pharmaceuticals and veterinary antibiotics. As such, the release of these chemicals into the agricultural environment remains largely unregulated. For chemicals with retained biological potency (e.g., pharmaceuticals), this is of particular concern because even at low environmental concentrations, the interaction of the chemical with a receptor has the potential to result in harmful effects on humans and non-target organisms.

A significant challenge remains in terms of how to address this risk, accounting for the sheer chemical diversity and complexity of emerging contaminants in an environment which itself is complex and dynamic. We need to harness the latest technologies and progress in high-throughput methods, trace residue analysis, and predictive toxicology to enable large-scale, fast, and accurate testing. Using these methods as a screening tool will ensure focused efforts on assessing the risk of contaminants of most concern. Solution-driven research to allow for the safe reuse of "waste" to land is only possible when we have a better understanding of the risks associated with these practices.

Carla A. Ng
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Revealing knowledge on fluorinated substances

Per- and polyfluoroalkyl substances (PFASs) include thousands of chemicals pervasive in many applications (e.g., stain/water-resistant fabrics, cleaning products, and fire-fighting foams). Their use has led to widespread human and wildlife exposure to what are, unmistakably, "novel entities" in the environment. Other than a handful of natural compounds, most PFASs have no natural origin, and several are known to be toxic at extremely low concentrations (consider the US EPA's *part-per-quadrillion* interim health advisory levels for perfluorooctanoic acid and perfluorooctane sulfonate). Moreover, known PFAS health effects span multiple biological systems. Yet mechanistic insight into the health effects of the entire structurally diverse PFAS class remains elusive, largely because public information is unavailable for most PFASs in active use. Despite intense public and scientific scrutiny, most data on PFAS behavior and toxicity are limited to fewer than 20 substances. The "unknown unknowns" of the use, identity, and properties of untested PFASs pose an enormous challenge to protecting humans and wildlife. Such information is critical to mitigate exposure by reducing non-essential uses, anticipate health risks for contaminated populations, and, ultimately, inform the design of safer replacements. Despite these data gaps, the extreme persistence of PFASs make environmental contamination essentially irreversible, carrying high costs should other damaging impacts become known in the future. Given this certainty, and a long history dealing with persistent halogenated substances such as chlorinated pesticides and brominated flame retardants, the need to move away from PFASs is clear and urgent.

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Toward improved risk evaluation for airborne chemicals

Assessing the environmental and human health risks posed by complex mixtures of airborne chemicals serves as the scientific basis for chemical management. Currently, effective risk evaluation is still stymied by two knowledge gaps: (1) a limited understanding of the airborne chemicals, including "What are they?" (i.e., the chemical structures), and (2) uncertainties regarding the chemical origin—i.e., "Where do they come from?"

The identified airborne chemicals so far likely represent the tip of the iceberg. This is partly due to the existing target-analysis approach to identifying airborne chemicals, which focuses on certain groups of targeted compounds. It is also a result of the immense analytical challenge associated with tracking "unknown compounds," for which no analytical standards exist. To evaluate the overall environmental and health impacts of airborne chemicals, including the unknowns, the development of advanced analytical techniques (e.g., non-target analysis) and authentic standards is urgently needed.

The challenge to understanding chemical origin is to illustrate the complex atmospheric chemistry of airborne chemicals. Specifically, during their residence time in the atmosphere, synthetic chemicals undergo reactions with oxidants such as hydroxyl radicals and ozone, leading to the formation of many structurally diverse transformation products. However, for most chemicals of emerging concern, little is known regarding their atmospheric reaction kinetics, transformation mechanisms, or oxidation products, thereby adding an extra layer of unknowns to the "unknown compounds." Including atmospheric transformation products in future contaminants monitoring networks will better inform the risk evaluation of synthetic chemicals.

Martina G. Vijver
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Opportunities in predicting "matter out of place"

Although we strive to direct chemical innvoation, we are increasingly encountering a lot of "matter out of place"—pollution created by synthesized chemicals and advanced materials (e.g., nanomaterials). It is by no means straightforward to assess where all the pollutants will end up and what ecological risks are induced. Persistent, bioaccumulative, and toxic substances, where unknown risks are surfacing, are causing the greatest concern. To realize a future of safe and sustainable chemicals for planetary health, there is still a window of opportunity if we can make things right from the start and address undesirable outcomes accurately and in a timely fashion.

The European Commission (EC) has taken the lead by launching a chemical strategy for sustainability to stimulate a transition to more safe and sustainable chemicals, as part of the European Green Deal. Pragmatically, this would ask for, e.g., replacing substances of concern with chemicals that are safer and investigating nanomaterials making use of the "green and clean" claim and phasing out the most harmful substances.

Clearly thus, the environmental assessment of synthetic and engineered materials must be scientifically and systematically scrutinized, e.g., assessing short- and long-term socio-environmental and health impacts as well as balancing costs. Additional progress can be made by adopting an integrated framework of prospective risk assessment and *ex ante* life cycle analysis, which will allow us to make safe and sustainable-by-design predictions. The future is always uncertain regarding unintended pollution and risks, but we must learn to take decisive prospective actions to protect ecosystems and their inhabiting communities.

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Safe and sustainable across scales

Several chemicals pose a threat to our Earth support system, prominently some persistent organic substances and plastics. More importantly, the wider realm of anthropogenically released chemicals essentially affects ecosystems at local and regional scales, contributing to the global threat. Achieving global reduction targets for chemical pollution must hence consider ecosystems' capacities to cope with chemical pressure at their respective scales. However, the ever-increasing diversity of chemicals, materials, products, and related regulations poses significant challenges for assessing and managing chemicals across scales. Interactions between technological systems, humans and the environment, and complex fate, metabolism, exposure, and effect mechanisms require a highly integrated and systems-level approach to address pollution from chemicals along their life cycles. In addition, temporal scales need to be acknowledged, from short-term chemical reactions to accumulation over decades or more. A vision for sustainable chemicals requires full circularity, with zero waste and pollution, but is currently hampered by mounting unknown toxicity of chemicals and their legacies across space and time. Solutions must move away from drop-in chemical replacements toward effective and sustainable alternatives adopting function-based substitution at chemical, material, and technology level. To move forward, we need to consistently integrate safety and sustainability thinking across scales, respect local-to-global biophysical boundaries, and innovate along the entire chemical value chain to offer a wider and viable solutions space to design safe and sustainable chemicals, materials, and products.

DECLARATION OF INTERESTS

L.C. has been appointed to sit on the Hazardous Substances Advisory Committee to provide comment to Defra on Hazardous Substances.