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CHEMICAL POLLUTION IN WATER: SCALABLE AND INTERSECTIONAL OPPORTUNITIES FOR THE ANALYTICAL AND SOCIAL SCIENCES

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Summary

Many anthropogenic chemicals now exist in our environment, but we still have insufficient information about their risks or impacts. There is an urgent need to increase the scale of capability to assess this planetary crisis. Here, we focus on important opportunities for cooperative and intersectional analytical and social science solutions.

The challenge of scale

Chemicals have undoubtedly enriched our lives, providing substantial benefits ranging from life-saving medicines to new materials in the latest fashions. In 2022, global chemical sales reached € 5.434 trillion, with China, Europe, and the USA accounting for 73 %[1]. The American Chemical Society's Chemical Abstracts Service Registry lists over 219 million chemicals reported in the literature since the 1800s and the rate of discovery is increasing. Of these, >350,000 are licenced for manufacture and use worldwide[2]. However, widespread contamination of the environment makes them a substantial component of the exposome. Some represent a 'hidden threat' to health, most notably regarding their potential for developmental neurotoxicity, reproductive toxicity and immunotoxicity. Pollution is now the largest environmental risk factor to human health and is estimated to be responsible for one in six premature deaths annually. Water pollution alone contributes 1.4 million deaths (second only to air pollution at 6.7 million) and 2.2 billion people still do not have access to safe drinking water[3]. Six planetary boundaries have now been exceeded including for "novel entities" in 2022[4].

Major routes for chemicals to water include contamination from agricultural and water treatment practices, leaching from containers or pipes, storm runoff and intentional release. Daily exposure occurs mainly through ingestion, dermal contact and vapour inhalation. To understand chemical risks at scale (i.e., their probability of causing harm), we first need to define the hazard (how dangerous they are) and the exposure (i.e., the concentration and whether it is chronic or acute). Surprisingly, though health impacts are well understood, legacy pollutants like lead remain an issue[3]. For most other chemicals, we know very little. For example, >600 disinfectant by-products have been identified in treated drinking water at low-sub microgram per litre concentrations and are formed from dissolved organic matter present in source water. Sub-groups of these (e.g., the trihalomethanes) have been associated with elevated bladder cancer risk[5], but causal links to individual compounds are still lacking.

Therefore, if water becomes progressively more polluted, the use of non-‘pristine’ or recycled sources therefore needs to be rigorously and regularly evaluated.

Policies and regulatory frameworks in several regions help protect health and the environment from chemicals in water. But in reality, many do not have enough reliable data to adequately assess the effects of chronic exposures individually, let alone when present as mixtures in reality. To exacerbate the problem, most chemicals are (bio)transformed into other compounds after consumption, including in the environment. This presents even more complexity, as transformation products cannot be assumed to be non-toxic. A rapidly growing body of literature (Figure 1), documents that more unregulated chemicals end up in our environment than we thought. In addition, water treatment technologies are not designed to eliminate all chemicals. We recently showed that of 58 pharmaceuticals and pesticides detected in surface waters, most were not entirely removed during wastewater treatment[6]. Policies, including bans, though often effective, do not always solve the issue and recent global conflicts have also impacted the chemicals industry further. Relocating manufacturing and/or transporting waste to less economically-developed nations, as well as market repositioning and ‘regrettable substitution’ remain challenging issues. For example, the neonicotinoid pesticide, imidacloprid, is banned in outdoor agriculture in the EU since 2018 because of its risk to bees and pollinators.[7] In the UK, market repositioning following the ban led to imidacloprid being used widely as a prophylactic ecto-parasiticide in companion animals. Environmental risks now exist in water, with major contributary routes emerging that were not as obvious previously, such as via urban wastewater.[8] Furthermore, it has been reported that large proportions of EU exports of neonicotinoids (including imidacloprid) have been sent to low- and middle-income countries, with the largest importer being Brazil.[9]

Intersecting analytical and social sciences

Many large initiatives are now underway such as the Global Framework on Chemicals, which recently set out 28 targets to improve the management of chemicals and waste, including multi-stakeholder engagement to phase out hazardous chemicals and development of sustainable alternatives. Within our own research fields of environmental chemistry and consumer behaviour, we perceive that important solutions lie at intersections between the analytical and social sciences. We identify selected themes that individually are already showing promise, including at large scale (Figure 2). Combining multiple themes would be a major step in the right direction, e.g., better and more comprehensive monitoring technology in the hands of Citizen Scientists to effect meaningful behavioural change. Understanding chemical pollution is critical (i.e., *where and when* it occurs, and *what* its impacts are) for policy, regulation and health protection, but also *why, who* and *how* we consume chemicals. Among all the pollution mitigation and environmental protection-focussed solutions, we argue that the value of research at these intersections has not yet been fully realised, especially for design and assessment of interventions. Such collaborative investigations could rapidly improve knowledge and wider awareness of chemicals risks.

Scaling up analytical approaches for chemicals

Occurrence of a chemical in water and potential for ecosystem impacts can be partly estimated using manufacturing and sales data when combined with toxicological information, if it exists, or can be predicted reliably. However, exact chemical ingredients in marketed products are not always available or openly accessible (e.g., to protect commercial interests) making this sometimes difficult. Evidence lies in actual measurements in water. This remains a substantial challenge where so many different chemicals could occur at trace concentrations. Laboratory capability has improved markedly, notably in the ‘omics fields, to make analysis more efficient and much more comprehensive for thousands of substances. For example, we used rapid mass spectrometry to extensively map the changing occurrence of large numbers of chemicals in Greater London’s waterways.[10] With global reach, Wilkinson and colleagues also recently applied similar methods to measure pharmaceuticals in >250 of the world’s rivers across all seven continents.[11] While maintaining quality, these approaches reduced the reliance on tedious laboratory sample preparation procedures and collection of large samples, thereby easing logistics and specialist training requirements. Moving out of the laboratory and into the field, low-cost autonomous sampling and sensing of trace chemical pollutants also present excellent opportunities for scaling up and now benefit from rapid prototyping tools such as 3D printing.[12] Their key challenge is in the provision of high quality, near-real time data, while withstanding changing environmental conditions for long periods of time. Furthermore, combinations of lower cost biological and chemical analysis capabilities together within such devices will undoubtedly make exposure evaluations much more accessible and useful.

With respect to (eco)toxicological testing of chemicals, ‘new approach methodologies’ (NAMs) aim to address the 3 Rs of animal testing, Reduction, Replacement and Refinement, and include *ex vivo*, *in vitro*, *in chemico* and *in silico* approaches. Progress to NAM adoption to replace animals in regulatory decision-making is advancing in many countries. In the age of ‘big data’, there has been a notable surge in the development of curated resources and modelling approaches for NAMs incorporating machine learning. There are recognised challenges to adopting these in particular, e.g., limited confidence in their ability to predict hazard class for some endpoints and validation. While the quality of evidence they provide still needs to be carefully evaluated, some have already outperformed animal testing approaches for chemical hazards.[13]

Lastly, experienced researchers have coordinated their efforts to enable exchange of knowledge internationally among groups, consortia and networks, which aim to coordinate and harmonise R&D as well as share, evaluate and promote ‘best practice’, and represent a ‘collective voice’. Data sharing, in particular, represents a key ‘living’ resource to help keep pace with continually evolving pollutant cocktails. An example is the NORMAN Network which has reported over 4,553 unique chemicals across a range of environmental media (>96 M data entries). In Europe, 1,474 chemicals have been reported in water above the analysis detection limit and for which supporting quality information is available (Figure 3). Another example, especially since its rapid scale-up during the COVID-19 pandemic, is the SCORE Network. This network undertakes collaborative wastewater-based epidemiology to monitor, among other things, community chemical exposure and health. For example in 2023, it characterised illicit drug consumption patterns for tens of millions of people simultaneously across 111 cities (85 % were within the EU). While a step in the right direction, limitations exist for such networks, such as compromises that need to be made regarding sustainability, quality assurance and transparency, especially regarding open access to data. Even with all these advances, *a priori* knowledge remains critical to help prioritise samples, groups of chemicals, or study sites and this limits larger scale coverage. Sampling and/or testing everywhere, for all available chemicals, and all the time is clearly not an option. This is where cooperation with the community and integration with the social sciences can help.

Community engagement and Citizen Science

A key trend among technological and methodological improvements for large-scale applications is the development of more efficient and user-friendly approaches, making them accessible to non-specialists.[10,11] This reveals another opportunity, i.e., scaling people-power to tackle the scale of the problem. The concept of community *engagement* is not new, but community *empowerment* to help design, execute, and evaluate scientific research for collective gain has garnered traction. Opportunities in Citizen Science have notably increased on a massive scale. Thousands of projects now exist globally and are embedded within industry, government agencies, higher education institutes, charities and community level groups which actively invite the public to engage in the scientific process to help discover new galaxies or find a cure for cancer. Regarding water pollution, an example is Earthwatch Europe, which in 2022 reported that it had already trained nearly 4,000 people to collect Citizen Science data over the past 10 years.[14] This includes the provision of field testing kits (e.g., for nutrient pollution), which have led to the submission of 2,200 new datasets to their online database covering >1,200 freshwater bodies and across 32 countries. Challenges still exist for Citizen Science, mainly regarding perceptions of the quality and value of data generated by non-specialists. However, better integration within formal monitoring programmes could prioritise locations for action more rapidly. Sustained cooperation with such groups will improve the collective knowledge of both Citizen Scientists and professionals alike, enabling more effective combination of their resources. But, and it's a big but, this requires funding, co-ordination, and more people on both sides to care enough to take action to drive wider impact. Therefore, it is not just about what we can collectively do to solve the problem, but what makes it important enough to motivate more of us to want to adopt a more proactive and shared approach.

Markets, ethics of care, and behavioural change

The power of marketing and persuasion to steer demand is immense. As more aggressive chemical restrictions emerge, marketers must invest in greener solutions or face an existential crisis for their business. A good example are per- and polyfluoroalkyl substances (PFAS) used in a huge range of everyday items due to their thermal stability, hydrophobicity and non-stick properties. Widespread occurrence and persistence of these "forever chemicals" has led to major health concerns including potential impairment of immune, thyroid, liver and kidney function, effects on lipid metabolism and insulin regulation, developmental and reproductive effects and even cancer.[15] Very tight regulation at such ultra-low concentrations is emerging with, for example, the European Chemicals Agency now considering restriction of ~10,000 PFAS. Well-known brands have already engaged in visible marketing strategy changes, including investing in PFAS alternatives for use in waterproof clothing, cooking equipment, and cosmetics, as examples. But it needs to go further. Marketing ethics need to be improved moving forward to evaluate the benefits of greener chemicals beyond capital gain and across their entire life cycle. Wider community engagement, including through corporate Citizen Science initiatives, is a welcome development. However, it is critical to avoid 'greenwashing', resulting in a dilute-and-divert Public Relations exercise, rather than meaningful co-operation with communities in pursuit of finding more responsible solutions.

Aside from the obvious expectations to improve practices and accountability of those responsible for chemicals governance, on aggregate, individuals and communities play an underpinning role in environmental protection and justice. The key point here is that individuals need to change their consumer behaviour and social science can inform strategies to better steer individuals in that direction and remove barriers to doing so. For example, we often consume according to what is available and accessible to us, including the products themselves, but also their waste solutions and advice/information about them. Without viable and obvious alternatives in place, how can we expect more individuals and communities to both care and change? For example, deeper and richer ethnographic research embedded within communities can generate a profound understanding of how and why they consume and dispose of chemicals in certain ways (and link these to structural, cultural socioeconomic inequities affecting behaviour). These insights can meaningfully intersect with large-scale chemical monitoring programmes (e.g., wastewater analysis and local support groups for illicit drug use). It is also worthwhile considering why people care and engage in sustainability initiatives in the first place, i.e., their own ethics of care.[16] Research has regularly shown that groups or individuals care about issues like environmental pollution, but mainly when a threat is imminent and direct, or when emotions or high capital risk is involved. Consequently, we rarely act entirely altruistically and how we care in practice is often conflicted, compromised and contextualised[17]. This is especially the case when the causes, consequences and impact timeframes are vague or unknown, as may be the case for chemicals in the environment. As long as caring is a choice, it will remain an option that some will be able to avoid. Any campaign aiming to switch on the ‘care factor’ should keep this in mind. Although a pertinent question may be to what degree individuals should be asked or required to care and be “responsibilised” for pollution and sustainability, an undeniable fact is that collective change is fundamentally important for all stakeholders.

In conclusion, analytical capability is ready to make a step change in its scale of application for chemical water pollution. Integration of disruptive technologies such as NAMs and other readily scalable initiatives such as Citizen Science present clear opportunities to assist with this, but with careful evaluation of the evidential quality they provide. Co-production and integration with deeper and more socio-culturally embedded qualitative research is needed to better understand *why* and *how* chemicals are consumed by diverse communities.

Combining both analytical and social science-based approaches can provide better evidence of the impacts of interventions, including behavioural change. If we are to tackle chemical pollution on the scale it demands, we all need to change. We must take a hard look at how we live, from being more aware of the environmental impacts arising from our mundane everyday consumption practices to who we vote for in government. It all affects our ‘chemical planet’.

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Author contributions

L.P.B. led the paper and wrote initial draft with W.H. A.K.R and L.P.B. generated the graphical components. All co-authors contributed to revising and improving the text.

Declaration of interests

The authors declare no conflicts of interest.

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Figure Captions

Figure 1. The number of Scopus publications over the past century focussing on chemical pollution in water, including selected classes. Data presented on $\log_{10}$ scale. Specific search terms are given in the key and no other filters were applied.

Figure 2. Overview of selected intersectional R&D themes within the analytical and social sciences. These could be combined to help better understand and anticipate the risks of chemical contaminants in water.

Figure 3. Collated data from the NORMAN Network EMPODAT database showing the number of all emerging substances identified to date above method detection limits in different water types across 25 European countries (n = 1,343,625 data entries; n = 1,474 unique substances across all water types). Compounds are known to be present in the environment, but not included in routine monitoring programmes. Note: the database does not include occurrence in drinking water and data from passive sampling-based studies is excluded. Only compounds with supporting quality-related information are shown.