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A path to clean water

Reduced chemicals input must complement wastewater treatment to ensure the safety of water resources

By Klaus Kümmerner¹, Dionysios D. Dionysiou², Oliver Olsson¹, Despo Fatta-Kassinos³

Chemicals, including pharmaceuticals, are necessary for health, agriculture and food production, industrial production, economic welfare, and many other aspects of modern life. However, their widespread use has led to the presence of many different chemicals in the water cycle (1, 2), from which they may enter the food chain (3, 4). The use of chemicals will further increase with growth, health, age, and living standard of the human population. At the same time, the need for clean water will also increase, including treated wastewater for food production and high-purity water for manufacturing electronics and pharmaceuticals. Climate change is projected to further reduce water availability in sufficient quantity and quality. Considering the limits of effluent treatment, there is an urgent need for input prevention at the source and for the development of chemicals that degrade rapidly and completely in the environment.

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LIMITATIONS OF WASTEWATER TREATMENT

Conventional wastewater treatment has contributed substantially to the progress in health and environmental protection. However, as the diversity and volume of chemicals used have risen, water pollution levels have increased, and conventional treatment of wastewater and potable water has become less efficient. Even advanced wastewater and potable water treatments, such as extended filtration and activated carbon or advanced oxidation processes, have limitations, including increased demand for energy and additional chemicals; incomplete or, for some pollutants, no removal from the wastewater; and generation of unwanted products from parent compounds, which may be more toxic than their parent compounds (5, 6). Microplastics are also not fully removed (7), and advanced treatment such as ozonation can lead to the increased transfer of antibiotic resistance genes, preferential enhancement of opportunistic bacteria, and strong bacterial population shifts (8).

Furthermore, water treatment is far from universal. Sewer pipes can leak, causing wastewater and its constituents to infiltrate groundwater. During and after heavy rain events, wastewater and urban stormwater runoff is redirected to protect sewage treatment plants; this share of wastewater is not treated. Such events, as well as urban

flooding, are likely to increase in the future because of climate change. Globally, 80% or more of wastewater is not treated.

INPUT PREVENTION

The limitations of treatment technologies call for more emphasis on input prevention. Pollution reduction at the source will allow water treatment to be more effective and efficient to meet quality objectives. When sufficient input prevention measures are available, end-of-pipe treatment can be more targeted and thereby more effective.

For industrial wastewaters, there are several components to this input prevention approach, including using fewer different chemicals in manufacturing; replacing nonbiodegradable with biodegradable chemicals; keeping water flows of different composition separate; and keeping auxiliary chemicals (which support manufacturing processes and are not part of the product) in closed loops for reuse and eventual recycling. Regulations supporting this approach include the U.S. Clean Water Act Amendments, which stipulate zero discharge promotion to reduce pollutant discharge.

Zero discharge has become effective, for example, in semiconductor and textile industries. In the best case, it enables recovery of auxiliary and product ingredients that did not end up in the product. For example, in the manufacturing of textile fibers and their processing, such as dyeing, some ingredients can be separated, purified by crystallization, and reused. In India, zero discharge is mandatory for textile and chemical industries. Many dyeing factories were closed down by the government a few years ago and allowed to reopen only once zero discharge measures were in place. Polluted waters are treated inside the factories; salt, for

Even modern treatment plants, such as this one in Sha Tin, Hong Kong, cannot remove all pollutants from wastewater.

example, is recovered and reused in dyeing, as are sizing chemicals and unused indigo from denim dyeing.

Separation at the source will be much more challenging for municipal wastewater, where it will require a focus on the chemicals used in products. This may involve selection of biodegradable compounds, use of fewer constituents, and use of smaller amounts of chemicals overall.

For example, organic silicon compounds were long seen as indispensable in shampoos. However, they do not fully degrade in the environment, and their degradation products are ubiquitous. Following increasing consumer awareness, producers have begun to promote silicon-free alternatives, saving money in the process because they require fewer ingredients. Similarly, replacing plastic microbeads with fully and readily mineralizable cellulose microbeads in cosmetics would avoid the release of long-lived microplastics into the environment. Given the numerous ingredients of cosmetic and other products, there should be many such opportunities for reducing the environmental burden of synthetic chemicals.

Recent developments in green (9) and sustainable chemistry (10), including pharmaceutical chemistry, also offer approaches for input reduction or prevention. One promising approach is to understand the reasons for use of a chemical substance, determine which functionality it offers, and explore nonchemical alternatives. For example, different construction or design of a building may eliminate the need for fungicides, if wooden parts are only used where water has no access. Similarly, different consumer behavior or alternative business and service-oriented models could reduce the amount or nature of chemicals used (11, 12).

BENIGN BY DESIGN

Even if input can be reduced, it is obvious that chemicals will continue to be needed, albeit perhaps in smaller amounts. Ideally, any such chemicals that remain in wastewaters should be designed such that they are rapidly and completely mineralized (degraded to carbon dioxide, water, and mineral species) in effluent treatment or even in surface waters. For example, linear alkyl sulfonate was developed for quick and complete mineralization over 50 years ago as a substitute for the persistent synthetic detergent tetrapropylene sulfonate. It is thus feasible to intentionally design chemicals in such a way that treatment or processes in the environment would lead to fast and complete mineralization (“benign by design”).

Accordingly, to be environmentally benign, the chemicals and products of the future must be assessed to meet this requirement at the very beginning of their life cycle, taking into account the end of their life even before their synthesis. There is limited chemical freedom to vary the core parts of molecules that are essential for their function. However, other parts can be varied much more to foster quick and complete mineralization in conventional wastewater treatments or aquatic environments (13). Encouraging examples are available even for widely used pharmaceuticals, such as β -blockers (14), and chemicals, such as ionic liquids (15).

GOING BEYOND INDIVIDUAL APPLICATIONS

Although examples of more benign chemicals exist, going beyond these individual applications requires improved knowledge and management of the substance, material, and product flows in the global economy. Knowledge of the local, regional, national, and global variations and dynamics of these flows would

help to identify opportunities and levers for reducing their chemical complexity. Better knowledge of products, their targeted design, and an enhanced understanding of the function they offer are key for achieving this goal.

The current trend is, however, in the opposite direction, with ever more complex products with diverse composition entering the market and hence the environment. It is thus crucial that incentives and regulation are in place to steer product and chemical development in a more sustainable direction. To achieve such a change in direction, external costs such as wastewater treatment or environmental cleanup costs must be taken into account in product price. For instance, a slight modification in the production process to increase revenue may result in substantial external costs for wastewater and drinking water management, and vice versa.

Regulations and incentives are needed to make this happen. For example, introduction of the European chemicals regulation REACH reduced the number of chemicals on the European market as manufacturers balanced registration costs against possible revenues. In the future, fast-track registration or prolonged patent lifetime could help to incentivize the development of new compounds designed for fast and complete mineralization in the environment. Chemicals that are readily mineralized in the environment need not be as extensively tested for effects in the environment, reducing costs and saving time.

REGULATION FOR INDIVIDUAL CHEMICALS

In an ever more complex and interdependent world, the precautionary principle in general, as well as with respect to chemical input prevention at the source, becomes more important. What's going on at the beginning of the pipe determines what leaves the end of the

pipe, not the other way around. The amendment of water regulations presents an ideal opportunity to promote source control and drive innovation. Yet sewerage charges, if in place at all, are typically applied to cover the costs for (re)building sewers and operating sewage treatment plants.

In some countries, for example in Germany, there is an additional fee for the release of water that does not meet certain quality criteria. These fees are measured by sum parameters such as chemical oxygen demand and nitrogen and phosphorus content. There are also threshold concentrations for organic halogens and metals such as mercury, cadmium, chromium, lead, and copper, based on their toxicity to fish eggs. This approach has been very effective for input prevention, resulting, for example, in reduced use or recovery of halogenated solvents. It could be extended to persistent organic compounds in general, including specific toxicity such as mutagenicity, genotoxicity, and endocrine-disrupting potential. Bans for long-lived pollutants will help to reduce concentrations of pollutants that contribute little to the utility of products.

However, given the ever-increasing list of chemicals that are introduced into the aquatic environment, attempts to assess harm and introduce thresholds will tend to lag new introductions. A preventive approach is therefore also needed. For example, giving companies relief from effluent charges if they use compounds from a list proven to be of low toxicity and readily mineralized—such as the abovementioned cellulose microbeads—could provide strong incentives for creating more sustainable products. ■

REFERENCES

1. E. S. Bernhardt, E. J. Rosi, M. O. Gessner, *Front. Ecol. Environ.* **15**, 84 (2017).
2. R. P. Schwarzenbach *et al.*, *Science* **313**, 1072 (2006).
3. A. Christou *et al.*, *Water Res.* **109**, 24 (2017).
4. O. Paltiel *et al.*, *Environ. Sci. Technol.* **50**, 4476 (2016).
5. C. K. Schmidt, H.-J. Brauch, *Environ. Sci. Technol.* **42**, 6340 (2008).
6. D. Hanigan *et al.*, *Environ. Sci. Technol. Lett.* **2**, 151 (2015).
7. F. Murphy *et al.*, *Environ. Sci. Technol.* **50**, 5800 (2016).
8. J. Alexander, G. Knopp, A. Dötsch, A. Wieland, T. Schwartz, *Sci. Total Environ.* **559**, 103 (2016).
9. J. A. Linthorst, *Found. Chem.* **12**, 55 (2010).
10. K. Kümmerer, *Angew. Chem. Int. Ed.* **56**, 16420 (2017).
11. United Nations Industrial Development Organization, *Global Promotion and Implementation of Chemical Leasing Business Models in Industry* (UNIDO, Vienna, 2016).
12. C. G. Daughton, *Sci. Total Environ.* **493**, 392 (2014).
13. R. S. Boethling, E. Sommer, D. DiFiore, *Chem. Rev.* **107**, 2207 (2007).
14. T. Rastogi, C. Leder, K. Kümmerer, *Environ. Sci. Technol.* **49**, 11756 (2015).
15. A. Hai *et al.*, *Green Chem.* **18**, 4361 (2016).

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CHEMISTRY

Regulate to reduce chemical mixture risk

Regulatory systems must better provide for risks from exposure to multiple chemicals

By **Andreas Kortenkamp¹** and
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Humans and wildlife are continuously exposed to multiple chemicals from different sources and via different routes, both simultaneously and in sequence. Scientific evidence for heightened toxicity from such mixtures is mounting, yet regulation is lagging behind. Ensuring appropriate regulation of chemical mixture risks will require stronger legal stimuli as well as close integration of different parts of the regulatory systems in order to meet the data and testing requirements for mixture risk assessment.

Until about a decade ago, toxicologists, risk assessors, and regulators regarded risks from chemical mixtures as negligible, as long as exposures to all single chemicals in the cocktail were below the levels judged to be safe for each chemical alone (1, 2). However, an increasing body of scientific evidence has challenged this notion, showing that a neglect of mixture effects can cause chemical risks to be underestimated (see the figure). International bodies such as the World Health Organization now acknowledge the need for considering mixtures in chemical risk assessment and regulation (3). This would align toxicological risk assessment with the clinical sciences and their long tradition of investigating drug-drug interactions. Yet, with few exceptions, regulatory systems around the world still focus overwhelmingly on single-chemical assessments, and the translation of scientific evidence about mixture effects into better regulation is extremely slow.

THE SCIENTIFIC BASIS

The most widely used concept to determine the common toxic effect of combinations of chemicals is dose addition (DA) (3, 4). DA assumes that one chemical can be replaced by an equal fraction of an equally effective dose of another without diminishing the overall combined effect. This may, for example, be the case for combinations of chemicals that exert their toxicity through similar mechanisms, such as by binding to the same receptor.

In one of the earliest predictive mixture studies, DA provided good approximations of the joint effects of mixtures of 50 aquatic toxicants in fish (5). This seminal paper created the conceptual basis for numerous laboratory studies with microbes, mammalian cells, rodents, and isolated human tissues. In these studies, DA proved to be an excellent tool for anticipating experimentally observed combination effects of up to 80 chemicals, including pesticides, industrial chemicals, food contaminants, cosmetics ingredients, and pharmaceuticals (6, 7).

The principles of DA imply that every mixture component contributes to the combination effect in proportion to its dose and individual potency, even when each component is present at levels below its individual effect threshold. This idea has been tested in several experimental studies. The results show that mixture effects occurred when each chemical was present at or below experimental NOAELs (no observed adverse effect levels) for single substances (8). NOAELs are used to derive regulatory limit values through division by an assessment factor, typically 100. Examples are Environmental Quality Standards (EQS) set under the European Water Framework Directive.

The suitability of such EQS for protecting against mixture effects has been tested. Combinations of 14 or 19 pollutants at EQS levels produced substantial toxic effects in microalgae, daphnids, and fish and frog embryos (9), at concentrations 100-fold or more below their individual NOAELs. A mixture of 15 chemicals at the concentrations found in human amniotic fluid altered thyroid hormone signaling and early brain development in *Xenopus* tadpoles (10).

Clearly, single-chemical risk assessments cannot capture such phenomena. Mixture risk assessment is needed for better protection of humans and the environment. Scientifically justifiable tools are available and ready for use in risk-assessment practice.

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