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The need for chemical simplification as a logical consequence of ever-increasing chemical pollution

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Widespread presence of synthetic chemicals throughout the natural environment, both abiotic and biotic, including humans, is a fact, and improved analytical techniques now demonstrate the presence of mixtures of hundreds if not thousands of synthetic chemicals and their transformation products in the environment. For most of these chemicals, data on their effects on humans, animals, or plants are missing. For the roughly 24’000 chemicals registered under REACh, for instance, the European Chemicals Agency recently reported that 88% of the dossiers reviewed in 2020 were incomplete, particularly with respect to long-term effects. Conversely, several prominent legacy compounds, such as polychlorinated biphenyls, phthalates or PFOA, have been intensely investigated and have been shown to affect multiple life functions, including reproduction. Accordingly, the chemical pollution problem is being considered as one of nine planetary boundary threats, yet the least well understood.

While the absolute magnitude of the problem remains largely unknown, we can look at trends. Doing so provides hardly any reason to believe that things will dramatically improve in the near future, although over 20 years have passed since the introduction of the Green Chemistry principles. While some hazardous substances such as persistent organic pollutants or mercury are now regulated by international conventions, monitoring in polar regions suggests that “concentrations of these substances in many Arctic top predators remain elevated and may no longer be declining”[1]. In the agrochemical industry, the development of new active ingredients was driven by the search for highly effective substances to reduce amounts used while replacing pesticides with high mammalian toxicity. This has indeed led to a decline in the potential for toxic impacts on mammals, fish and birds, but the potential for impacts on pollinators, aquatic invertebrates, and terrestrial plants has increased over the same time period of 25 years[2]. Furthermore, a trend toward incorporating aliphatic carbon-fluorine moieties – the strongest single bond in organic chemistry –, not only in commodity chemicals, but also in agrochemicals and pharmaceuticals, suggests that also the problem of persistent chemicals will remain if not worsen. Finally, there are cases where the replacement of problematic substances has, in hindsight, been found ineffective or to even aggravate risk, such as the replacement of bisphenol A by slightly structurally modified bisphenols or the substitution of polybrominated diphenyl ethers with organophosphate flame retardants.

Why are all of these things happening although legislation requiring chemical risk assessment is in place in many countries? We argue that there are two major reasons for that: the sheer number of chemicals in commerce but also their rates of increase, and the complexity of the interaction between chemicals and biological systems. First, estimates of the number of chemicals in commerce vary from the roughly 100’000 chemicals in commerce in the EU before REACh, to the currently roughly 25’000 chemicals registered under REACh, up to a recent estimate of approximately 350’000 chemicals being marketed globally. While the number of chemicals in commerce thus remains somewhat unclear, temporal trend analysis for active substances indicates that the rates with which the number of substances increases is on par with, if not faster than, the rate of increase of the global gross domestic product[3]. The problem is further aggravated by the fact that chemicals in commerce often are transformed into a number of transformation products, typically even less well known, as they reach the environment. As a consequence, the speed at which the global market of chemicals increases outpaces the capacities for chemical risk assessment.

One could argue that all we need is to develop sufficiently good models to predict, rather than experimentally test, chemical risk and that this would speed up things considerably. However, this is where the complexity of the problem, i.e., the need to predict interactions between thousands of chemical moieties with thousands of biological targets, and to extrapolate these predictions to cells, organisms, populations, and even ecosystems, becomes overwhelmingly large. Prominent examples are attempts to predict microbial biotransformation or modes-of-action in ecotoxicology. While the principles were laid out more than 10-20 years ago, models that can be deemed accurate enough for chemical risk assessment are still scarce or have extremely narrow applicability domains.

What is the consequence of the above outlined state of the environment, regulation and science in our field and how can we achieve a more positive future trajectory? We propose that we need to seriously consider “chemical simplification” as a future goal of innovation in chemical science and industry for the problem to become tractable. Importantly, we present this consequence not as a political position, but we see it as a logical implication that cannot be ignored at this point in time when it has become evident that decades of extensive research into risk assessment methods in combination with new and more ambitious regulation have not been able to solve the problems of chemical pollution.

We envision two cornerstones of "chemical simplification". First, we concur with Kümmerer et al. (2020), who suggest that the number of chemicals used in many products, in particular in consumer products, needs to be reduced[4]. This would directly reduce human and environmental exposure on a large scale and is also essential for achieving the goal of a circular economy: materials that are designed for recycling need to be chemically simple. Second, grouping approaches should become an integral part of chemicals assessment. Grouping makes it possible to estimate the potential risk of chemicals with insufficient data by comparing them to chemicals from the same class with full data sets and complete risk assessments. Importantly, grouping helps to avoid regrettable substitutions by highlighting cases where suggested substitutes have similar hazard profiles as well-studied chemicals, and it supports phasing out hazardous chemicals from non-essential uses without the need for detailed risk assessments[5]. Grouping thus has the potential to facilitate the move towards a simplified and reduced portfolio of chemicals, which would make available money and efforts for conducting thorough risk assessments for those chemicals remaining in commerce.

At first, the idea of "chemical simplification" might sound like a step backward rather than forward. We think that the opposite is the case as putting the idea into practice calls for a lot of innovation in science and engineering. The concept of grouping, for instance, requires a thorough understanding of how chemical structure affects fate and effect of chemicals, and hence a reinforcement of chemical principles in environmental chemistry and toxicology that is still underexploited under the current testing paradigm. Similarly, developing chemically less intense, but functional materials and products requires intense development efforts and new design principles. Importantly, this also offers promising market opportunities because materials and products that are easier to recycle and inherently safe are in high demand by many large brands of consumer products and by the consumers themselves. Innovative solutions can always be protected by patents, irrespective of the type of chemistry they contain. With this viewpoint, we hope to initiate follow-up discussions on how to innovate chemicals, chemical products and chemical assessment towards simplicity, efficiency and environmental safety.

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Short biography Kathrin Fenner

Dr. Kathrin Fenner is Associate Professor of Environmental Chemistry at the Chemistry Department of the University of Zurich, Switzerland, and a senior scientist and group leader at the Department of Environmental Chemistry at the Swiss Federal Institute of Aquatic Science and Technology (Eawag). Her research focuses on experimental and model-based approaches to gain an in-depth understanding of chemical persistence in the environment. The goal of her research is to not only improve current hazard assessment schemes but also provide tools and design principles for better degradable compounds and efficient approaches to bioremediation. In 2015, she received an ERC Consolidator grant to support this line of research. She has published more than 90 scientific research articles in the field of environmental science. Kathrin chairs the section of "Chemistry and the Environment" of the Swiss Chemical Society, has been member of several ECETOC expert groups and is currently Associate Editor with Environmental Sciences: Water Research & Technology.

Short biography Martin Scheringer

Dr. Martin Scheringer is a professor of environmental chemistry at RECETOX, Masaryk University, Brno, Czech Republic, and a senior scientist and group leader at the Swiss Federal Institute of Technology (ETH) in Zürich, Switzerland. He has worked in the area of chemical hazard and risk assessment for more than 25 years with a focus on persistent organic pollutants and environmental long-range transport of organic chemicals. In addition to his scientific research, Martin Scheringer has worked extensively at the science-policy interface. He is a founding member of the International Panel on Chemical Pollution, IPCP, and a member of the Global PFAS Science Panel (GPSP). He was a co-author of the chapter on chemicals and waste in UNEP's 5th Global Environment Outlook (GEO-5) and has published three books and more than 250 peer-reviewed scientific publications. From 2015 to 2020 he was an Associate Editor of Environmental Science & Technology.