Synthetic Chemicals in the Environment

Insights from the Royal Society Global Environmental Research Committee

This paper is an output of a discussion on synthetic chemicals in the environment at a Royal Society Global Environmental Research Committee (GERC) meeting. It seeks to highlight science issues of interest to researchers, funders and Government.

Introduction

Chemicals are all around us in everyday life and provide many societal benefits. As well as those present in end products, many others are used as intermediates in industry. Estimates vary as to how many chemicals and formulations are on the market in Europe, but it has been estimated at around 80,000, with fewer having been rigorously tested for effects upon human health. Legacy chemicals such as PCBs and lead show that injudicious use of chemicals, although considered an asset at the time, can cause problems for human health and the environment long after use has ceased. It is important to know how substances enter the environment, their pathways within it, and their potential for effects on human health and the environment. Ideally, regulation should take account of all these factors, as well as production volume, and where possible, assessments should be undertaken before chemicals come into use. There is a strong case for the UK to take a new proactive approach to regulating chemicals in the UK that embraces new technology. Further development of a positive approval process to account fully for both societal benefit and risk should be considered. There are differing opinions as to whether chemicals regulation should be based upon hazard (i.e. the potential to cause harm), or risk (the probability of harm occurring). The latter, although requiring far more data for decision making is likely to be more permissive. On the other hand, a purely hazard-based approach might prove excessively precautionary and deprive society of valuable products.

Much of the difficulty of chemicals regulation arises from the massive range of both physicochemical properties and toxic mechanisms exhibited by chemicals. The former will determine environmental pathways and persistence, and the latter will identify those organisms at greatest risk of harm. Indirect effects, such as the toxicity of metabolites and the impact of chemicals upon antimicrobial resistance also require consideration. Protection of the environment does not guarantee the safety of humans and *vice versa*.

Whilst the appropriate regulation of chemicals is without doubt an area of complex policy choices, we provide here some insights to help further develop and deploy a balanced regulatory approach.

Research priorities

Areas identified as needing further intensive research include the following:

1) Improved numerical models capable of predicting the physicochemical properties of compounds based on their molecular structure. The behaviour of chemicals in the environment, including for example, their tendency to bioaccumulate is dependent upon fundamental molecular properties such as vapour pressure and water solubility, as well as related parameters such as the Henry Law coefficient and octanol-water partition coefficient. For substances entering the atmosphere, the rate coefficients for reaction with hydroxyl and nitrate radicals may determine their lifetime. Measurement of these properties are time-consuming and expensive, but while theoretical methods based upon

molecular structure or extrapolation are much faster, they currently often lack the accuracy needed to make sound predictions.

2) Developed numerical models capable of predicting environmental pathways, lifetimes, and exposure concentrations. Models have long been available which predict the partitioning of organic chemicals within environmental media, and in some instances, these are good predictors of environmental behaviour and concentrations. However, they are not universally applicable with good outcomes, and are not readily applicable to inorganic chemicals which present greater challenges for prediction. Environmental media such as soils present such a high level of variability as to make reliable prediction difficult, but generic characterisation of behaviour should be possible.
3) Methods which are able to predict the toxicity of a chemical to a wide range of organisms and target organs based upon analogy with others (e.g. genomics, lineage and traits), or the molecular structure and properties. Current testing is limited to a very small range of organisms easily handled in the laboratory, and testing on a wide range of live organisms would be neither practicable nor ethically acceptable. Genetic determinants of sensitivity have yet to be elaborated in detail, but some read-across based upon genotypic and phenotypic properties is possible. There is also much scope for the application of biomarkers and omics methods to elucidate the basic mechanisms of toxicity which could then be applied to prediction of sensitivity. Development of *in vitro* methods and their relation to *in vivo* responses would be a great asset.
4) Enhanced monitoring of humans and the environment. This can play a number of important roles. Rapidly increasing trends in concentration may be an early warning of problems to come. Wide range screening of contaminants can identify newly emerging threats, alerting the need for action. Sensors which determine specific fractions of chemicals, such as the available (as opposed to strongly bound) metal and the lipid-soluble fraction may have a role to play. Ultimately, if large datasets are accumulated in combination with ecological surveys, it may be possible to use machine learning methods to identify those components causing stress to the biota. The American NHANES survey is a good example of human biomonitoring which has revealed important associations between exposure and health.

Cross-cutting issues

1) A full life cycle and systems approach is essential. They should take account of vital issues such as the formation and toxicity of decomposition products and metabolites. Chemical exposures are normally to mixtures, and this needs to be accounted for, as well as the frequent presence of other stressors such as drought, temperature and microbial pathogens.
2) There is a need for assessment of the areas of greatest uncertainty so that limited resources can be focussed upon the topics of greatest need. The possibility of grouping chemicals for evaluation, and the associated uncertainties, need to be evaluated.
3) There would be benefit in a rigorous assessment of the consequences of using hazard versus risk as the criterion of acceptability. This would consider the balance of risk and benefit to society.