Sustainable chemicals

The right choice for the future

Benign by Design
Interview with Professor Klaus Kümmerer
For some it means a chemistry set when at primary school, for others (like me, for example) it is the fascination of studying it – chemistry is exciting with its many facets, uses and possibilities. At the same time, since the 1970s at the latest, we have been debating the dangers of harmful substances to human health and the environment. The Oeko-Institut has been working on this issue since it was founded. Both in the book “Chemie im Haushalt” (Household chemicals), to which Rainer Griesshammer made a major contribution and which was instrumental in raising public awareness of toxic chemicals in the garden, home and office as early as 1984, and in studies such as that into the lead poisoning of the environment in the Harz mountains in 1980, our scientists flagged up the effects of pollutants and contaminants early on, and have pressed for the sustainable use of chemicals.

We have now moved on a stage: it is no longer a matter of denouncing this week’s worst substance. Instead we are trying to find the best possible way to identify hazardous chemicals used in chemical industry and to replace them. The aim is to achieve the “sustainable” use of chemicals. In this issue of eco@work we will be explaining what that means exactly, what has to be done and the areas in which we have already seen some success but still see the need for improvement. We can also see that it is a matter both of identifying especially critical substances and of pinpointing opportunities and innovation gaps for chemical engineering. This is because, applied correctly, it can help us to use raw materials efficiently and to manufacture products which themselves help to save energy and resources.

In our view, it is particularly important when going down this route to produce good policy guidelines on the use of chemicals in industry. The aim of these would be to avoid the risks that can emanate from chemicals and to improve the properties of these chemicals so that they are environmentally, socially and economically viable. It goes without saying that these issues can no longer be resolved on a purely national level, but require European or other international agreements. Provisions of this sort include REACH, the European chemicals regulation, and the Stockholm Convention on persistent organic pollutants, which we will be telling you about. In both cases our scientists have contributed their expertise to the regulatory frameworks.

I hope you enjoy eco@work. Have some great days out in the country this summer,

Michael Sailer
CEO, Oeko-Institut
m.sailer@oeko.de
Professor Kümmerer, what is the story behind the Benign by Design initiative?

At the heart of this initiative is the question: How can we design a chemical substance so that it degrades rapidly and completely when it eventually gets into the environment? A lot of chemicals used in detergents and pharmaceutical products still get directly into soils, water bodies and the air. Benign by Design is intended to prevent the manufacture of any chemical substances that later deposit trace contaminants, known as micropollutants, in our environment. This is done by exact analysis of their relevant properties.

How do you go about this?

There are two different approaches. Chemical substances have a specific structure, you see, and thus certain properties – such as their solubility in water. In one part of our research we examine the structural elements of chemicals, or to put it more simply, their characteristic components, the properties of these elements and their relationship with one another. Comprehensive information on the structural elements is stored in a computer data bank. So, if you want to analyse a chemical substance, this data bank can use the structural formula to analyse the individual structural elements and specific characteristics and test which interactions occur between them. We can use that to investigate whether this substance is toxic or readily biodegradable. So, from a large quantity of data we deduce the properties of a particular molecule, that is to say of the chemical substance, and at the same time make use of the structure-property relationships.

What about the second approach?

That concerns the method known as docking. In this approach we look at the individual molecule in terms of its effects – for example in the environment – and can analyse its effectiveness for particular tasks. At the same time we might test whether a substance could work as a pharmaceutical drug.

How do you obtain the data needed for the analysis?

Our database is constantly developing. We get our data from various sources, such as scientific publications and also from the European Chemicals Agency (ECHA). Unfortunately the data that we get often isn’t specific enough – we might find out whether a substance is readily biodegradable, but not what sort of tests were used to establish that. That is why we carry out some tests of our own to improve and expand our database.

What can the procedure be used for?

Primarily for evaluating existing substances. REACH, the EU regulation on chemicals, also permits the use of computer-aided processes to collect data. And, of course, this procedure is especially valuable in new development, because we can use the database to identify specific properties of a substance prior to its manufacture.

Do you work with industry as well?

Oh yes, definitely, and I think it’s very important to exchange ideas with users. After all, what good is a product that is fantastically biodegradable but just can’t be used? I would like to work even more closely with industry, because this practical contact is obviously extremely important and of great value.

Thank you for talking to eco@work.

Interview by Christiane Weihe.

Klaus.Kuemmerer@uni.leuphana.de

www.oeko.de/132/interview01

Talking to eco@work: Professor Klaus Kümmerer, Professor of Sustainable Chemistry and Material Resources at the Leuphana University of Lüneburg.

“We can identify specific properties of a substance prior to its manufacture”

Chemical substances should be harmless to both human health and the environment. Best of all they should be harmless from the moment they come into existence – “benign by design”. Professor Klaus Kümmerer is working on the entire life cycle of chemicals at the Leuphana University of Lüneburg. He looks at the characteristics of familiar substances and uses these properties for newly-developed substances. At the same time he studies their degradability in the environment after use. In his interview with eco@work Professor Kümmerer explains the methods that can be used to analyse the positive and negative properties of a substance prior to its manufacture.
Use the good ones.
Avoid the problematic ones.
How can chemicals be sustainable?

We can’t have sustainability without chemicals! Coatings for wind turbines or modern insulation panels for innovative insulation systems – either way, chemicals often make an indispensable contribution to sustainable development. Yet when people hear the word “chemicals”, the first thing they think of is the negative impacts: polluted waters, burns to the skin, irritation of the airways. There are still many substances that deserve their poor reputation and which the Oeko-Institut experts would also like to see banned. But which are the really harmful chemicals and which are the “good” ones? And how do you recognise them?

Nowadays chemicals are used in all fields – including in those that are particularly important for a more sustainable future. They are used in building insulation as well as in solar modules and for efficient use of resources. “Sustainable chemicals are needed in all sectors of industry,” explains Professor Dirk Bunke from the Oeko-Institut, “and there are a lot of chemicals that have no negative impacts on human health and the environment and can be used without any problem”. By this he means chemicals such as readily degradable tensides for detergents based on renewable resources, which are only mildly toxic to aquatic organisms. “However, there are still a lot of chemicals that are extremely harmful to human health and the environment,” continues the Oeko-Institut’s specialist, “such as perfluorooctanesulfonic acid, PFOS for short. It still occurs in some types of surface coating but should not be used any longer owing to its harmful properties”.

In Professor Bunke’s view, just the fact that acceptable alternatives such as alkyl sulfonates exist is an argument for a complete ban on PFOS – even though it means adjustments for the businesses affected.

Chemicals that are used with sustainability in mind can also have negative impacts on human health and the environment. One of these is hexabromocyclododecane (HBCDD), a flame retardant used in thermal insulation. “There is an urgent need to develop innovative thermal insulation systems that do not rely on these dangerous chemicals”, says Bunke. That is because HBCDD is persistent, bioaccumulative and toxic at the same time – a PBT substance. “That means that the chemical is slow to degrade, accumulates in the body and in addition is highly poisonous to humans”, explains Bunke. Other especially problematic chemicals are the vPvB substances, which are very persistent and very bioaccumulative.

But how can businesses and consumers too distinguish between “good” and “problematic” chemicals? And how can they assess a suitable alternative? “In smaller businesses in particular there is often insufficient experience when it comes to selecting the right, that is to say the sustainable chemicals”, says Dirk Bunke, who is in charge of Sustainable Chemistry at the Oeko-Institut. Help is available in the form of a guide that the Oeko-Institut has produced jointly with the Institute for Environmental Strategies (Ökopol) for the German Federal Environment Agency. Under the heading “Sustainable Chemicals” it lists eight substance-related and seven use-
related criteria for evaluating sustainability. “A number of different factors are involved here”, explains Bunke. “As far as the substance is concerned these are its risks to human health and the environment, and also the greenhouse gas emissions and consumption of resources during manufacture, whereas factors related to use might include substitutability and innovation potential”.

The guide explains the individual criteria for assessing sustainability in detail and also formulates ten golden rules that can be used as guidelines for sustainable chemicals management. It recommends avoiding chemicals on the lists of problematic substances – this refers to the persistent organic pollutants (POPs) listed under the Stockholm Convention (see article “POPs and candidate substances” on page 8 for more detail). “If businesses avoid particularly critical substances when making their selection, they can be sure they are moving in the right direction in the medium term”, says Bunke, “because they can assume that sustainable substances will still be available to them for years to come”. Moreover, if possible we should only use the substances that are not harmful to health, are not dispersed widely, are not bioaccumulative and do degrade quickly in the environment. “That won’t work in all cases”, says the Oeko-Institut expert, “but the use-related criteria in the guide also help in cases where replacing substances is almost impossible because suitable alternatives aren’t available yet”.

The first stages of a sustainability check are quick to carry out. What takes longer is the comprehensive testing of a substance, i.e. a study of its complete life cycle. “That is why we have to prioritise when we do this”, says Professor Bunke. However, in the case of a company’s most-used substances (in terms of quantity) it can be worthwhile to examine whether they are available based on renewable resources, or whether transport routes, energy and water consumption can be reduced. On top of the classic issues such as pollution control and health and safety at work, adherence to rigorous social and environmental standards among suppliers and throughout the manufacturing company is also an important aspect determining the sustainability of chemicals.

The sustainable chemicals guidelines focus on examining individual substances and their applications. “The recommended criteria should be as simple as possible to apply and should also give small and medium-sized businesses confidence in their choice of chemicals”, explains Professor Bunke. On the other hand, the studies in which complete processes and technologies are compared on the basis of their sustainability go far beyond this – for example, photovoltaic modules made from disparate materials, and coating processes with or without fluorinated chemicals. Such probing questions demand an integrated study that presents the various aspects of the evaluation in a transparent manner. “In an analysis of this kind we have to look at savings in energy and materials, impacts on health and potential consequences for the environment, and balance them against economic and social opportunities and risks”, says Bunke. “This enables us to come up with recommendations that are comprehensible and backed by science. The professor and his team at the Oeko-Institut have developed a methodology for integrated assessment, which uses environmental life-cycle assessment methods as well as socio-economic analyses and standard assessments of human toxicology and ecotoxicology.”
REACH

REACH, the European regulation on Registration, Evaluation, Authorisation and restriction of Chemicals, entered into force in 2007. As well as the protection of human health and the environment its central aims are to guarantee free trade of chemicals on the internal market and to promote competition and innovation.

The regulation seeks to improve the information situation in relation to chemicals and puts the onus on chemical manufacturers and importers: they may not place any chemicals on the market without registering them with the European Chemicals Agency (ECHA). The data collected in the course of this depends on the quantity of chemical; for example, manufacturers and importers have to produce a safety assessment for quantities exceeding ten tonnes per year. However, users of the chemicals also have to show that they are handling substances and mixtures safely.

All chemical substances on the European market will have to be registered by the middle of 2018. In addition, REACH includes the possibility of declaring a restriction on chemicals with unacceptable risks and of compelling substances of very high concern (SVHCs) to be authorised (for more on this see the "Socio-economic analysis" information box and the article "POPs and candidate substances" on page 8).

The prohibition of a chemical can impact on economic growth and competitiveness as well as on employment. That is why the European regulation on chemicals (REACH) provides an instrument of socio-economic analysis (SEA). This can be used to assess the impacts of chemicals and the corresponding risk management on humans and the environment as well as the effects on society and the economy.

A socio-economic analysis can be used in authorisation or restriction procedures (see "REACH" information box). It can be produced in the authorisation procedure as part of an authorisation application for a substance of very high concern (SVHC). According to REACH, companies can obtain a specific authorisation for a substance of this kind if they provide proof of appropriate management of the risks to human health and the environment. If this is not possible, an authorisation can be issued only if the socio-economic benefit of the application exceeds these risks or if no viable alternatives are available. Businesses can produce a socio-economic analysis as evidence of this.

In addition, any proposal by a member state for the restriction of a substance can be supported by this instrument, since socio-economic impacts must also be taken into account in restriction procedures. The analysis should then include a systematic comparison of all possible risk management measures and an evaluation of the cost-benefit ratio of the restriction.

The European Commission takes the decisions on authorisation and restriction. It is supported in this by the Committee for Socio-economic Analysis (SEAC) at the European Chemicals Agency, which comments on each application.

Socio-economic analysis

The prohibition of a chemical can impact on economic growth and competitiveness as well as on employment. That is why the European regulation on chemicals (REACH) provides an instrument of socio-economic analysis (SEA). This can be used to assess the impacts of chemicals and the corresponding risk management on humans and the environment as well as the effects on society and the economy.

A socio-economic analysis can be used in authorisation or restriction procedures (see "REACH" information box). It can be produced in the authorisation procedure as part of an authorisation application for a substance of very high concern (SVHC). According to REACH, companies can obtain a specific authorisation for a substance of this kind if they provide proof of appropriate management of the risks to human health and the environment. If this is not possible, an authorisation can be issued only if the socio-economic benefit of the application exceeds these risks or if no viable alternatives are available. Businesses can produce a socio-economic analysis as evidence of this.

In addition, any proposal by a member state for the restriction of a substance can be supported by this instrument, since socio-economic impacts must also be taken into account in restriction procedures. The analysis should then include a systematic comparison of all possible risk management measures and an evaluation of the cost-benefit ratio of the restriction.

The European Commission takes the decisions on authorisation and restriction. It is supported in this by the Committee for Socio-economic Analysis (SEAC) at the European Chemicals Agency, which comments on each application.

Yet, even if it may be possible to ban substances of very high concern (SVHCs) in future, the fact remains: not all chemicals in use can be completely safe. “A lot of the functionalities that chemicals can produce will always be needed,” says Dirk Bunke, “but there is also a whole variety of tools for finding a truly sustainable solution in individual cases. They range from a single-substance-based risk assessment of a chemical and a socio-economic analysis of its applications to a portfolio analysis of an entire industrial company”.

Christiane Weihe
d.bunke@oeko.de
www.oeko.de/132/infocus1

CH₃(CH₂)ₙSO₃H

Alkyl monosulfonates
Readily degradable base materials for surfactants
POPs and candidate substances

Monitoring and banning hazardous chemicals

In total the Chemical Abstracts Service (CAS) of the American Chemical Society has registered over 71 million chemical substances so far, and many more are added every day. Some of these substances have never even left the laboratory where they were created, while we come into direct contact with others daily: they are in clothes, furniture and mobile phones as well as in pharmaceuticals and cosmetics. Many chemicals are safe or are used only in closed systems, but there are also particularly problematic substances that can be dispersed and in doing so cause long-term harm to humans, animals and the environment. These need to be identified and their use restricted or even prohibited. Environmental and human biomonitoring programmes help to observe and provide evidence of the impacts of these substances.

Every day chemicals are released into our environment – either through their direct use or through the use of products which contain them. These chemicals can get into the air, the water cycle, the soils and foliage, and the blood circulation of humans and animals. But which substances have the potential to be dispersed, to accumulate in the body and cause toxic effects? A number of different programmes on environmental and human biomonitoring provide information about these, one of which is the German Federal Environment Agency’s Environmental Specimen Bank. This regularly expanded archive of human and environmental samples began its continuing work in 1994, with the oldest specimens stored originating from as long ago as 1981. “Samples are taken at regular intervals from various species in fourteen different ecosystems such as rivers, forests and conurbations”, explains Rita Gross, a researcher at the Oeko-Institut. “So things like the leaves of beech and poplar trees, earthworms and feral pigeons’ eggs are tested annually”. People also come under scrutiny, however: every year blood and urine samples are taken from around 480 students. This process allows the dispersal of numerous chemical substances to be monitored and assessed over a long period.

Oeko-Institut experts are currently also involved in research into the results of environmental monitoring programmes. In collaboration with the consulting firm BIPRO and the Hochschule Darmstadt University of Applied Sciences, they have carried out a study for the Federal Environment Agency (UBA) into how these findings can be better used as a source of information for exposure estimates and risk assessments in the context of REACH, the European regulation on chemicals (see information box on page 7). “To do this we scrutinised different programmes and analysed whether they can help to fulfil REACH tasks such as the registration and restriction of chemicals”, explains Rita Gross. And the result? Yes, they can. “Many of these programmes can provide data for REACH”, she continues, “although more substances would need to be added and it should be made easier to access the corresponding data”. In addition to that, EU-wide activities need to be harmonised and expert exchange between chemicals assessors and monitoring specialists should be intensified. “We have also produced a guide outlining how the environmental monitoring data can be used for REACH”, says Rita Gross.

Monitoring programmes help to keep a check on chemical pollution affecting human health and the environment. But which are the substances needing strictest observation? They include PBT...
and vPvB substances (see also page 4 “Use the good ones. Avoid the problematic ones”), the CMR (carcinogenic, mutagenic and toxic for reproduction) substances and endocrine-disrupting substances. “These chemicals affect the hormonal system,” says Rita Gross, “and include nonylphenol, which is used in paints and varnishes, for example, and bisphenol A, which is used in the manufacture of plastic packaging and has been found in food”.

The restriction or prohibition of especially problematic substances is implemented both in the context of REACH through the candidate list and through the global Stockholm Convention on persistent organic pollutants (POPs). The candidate list contains substances of very high concern (SVHC). However, prohibition only takes effect if they are listed in Annex 14 of the REACH regulation, for which prioritisation criteria such as widespread use and use in large quantities must be met. Even then companies can still apply for authorisation of a substance under certain conditions. In the context of the POPs convention there are currently 22 chemicals listed that accumulate in the body and, after release, are dispersed worldwide via air and water, as well as via the food chain, affecting people and the environment far away from the point of release. Their manufacture and use is restricted or even prohibited by the Stockholm Convention. POPs include amongst other things pesticides such as DDT and chlordecone and also industrial chemicals such as polychlorinated biphenyls (PCBs) and commercial octabromodiphenyl ether (C-octaBDE). PCBs were used mainly in open applications such as joint sealants and in capacitors and transformers, while C-octaBDE was utilised in such things as computer and television housings.

In a further study for the Federal Environment Agency, the Oeko-Institut worked with the Swiss Federal Institute of Technology Zurich (ETH Zurich) to analyse how potential POP candidates can be identified. In addition the scientists examined the data and processes which were used to identify existing POPs. “The aim of the study was to systematise the proposing of a chemical for the POPs list with reference to national, European and international levels”, explains Markus Blepp from the Oeko-Institut. For this the researchers developed a multi-level process which sets out two key stages: the examination of the substances using the listing criteria given in the Stockholm Convention, such as their potential to be transported over a wide area, and a specific evaluation of further information about the chemical, such as about its use and quantity, its negative impacts and its legal significance. “This forms the basis for including POP candidates in the Stockholm Convention assessment procedure or for specifically driving forward the extension of the list”, says Blepp. This is an important stage on the path to a global ban on substances of very high concern. Travelling that path serves to protect human health and the environment from those substances that are permitted to leave the laboratory – despite being harmful.

Christiane Weihe
r.gross@oeko.de
www.oeko.de/132/infocus2

**Suspect groups**

Ban one substance and so achieve effective protection? Sometimes this is no use because, if a substance belongs to a group of chemicals in which the other members exhibit the same hazardous properties, banning an individual chemical has often led to its replacement by another member that is no less hazardous. That is why the Oeko-Institut supports the notion that in such cases the relevant bans should apply to the whole group of chemicals.

This applies to substances such as halogenated flame retardants used in insulation materials and plastic casings. For example, brominated flame retardants like polybrominated diphenyl ethers, hexabromocyclododecane and tetrabromobisphenol A have exhibited critical effects. The use of these substances and other halogenated flame retardants, whereby very critical combustion products can arise, should be prohibited collectively instead of individual chemicals being banned. Through its research the Oeko-Institut is supporting companies which are developing and applying alternative substances.