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Abstract

Environmental and health problems caused by chemical pollution, especially high-risk chemical pollution, have become an important factor affecting the public health. How to ensure that chemicals bring well-being to human society, while ensuring that they minimize their harm to the environment and human health, is a problem that needs to be solved urgently in the field of chemistry, especially environmental chemistry. This article summarizes the latest research progress in the risk identification, risk prevention, alternative research and development and evaluation of perfluorinated compounds and other substances, and systematically explores how to use green chemistry, combined with the risk management and control, to decrease the risk of the high-risk chemicals during their entire life cycle. The article also discusses the research progress, development direction, and future development of high-risk chemicals throughout the life cycle.

Keywords

risk assessment; alternatives; green chemistry; life cycle

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Abstract: Environmental and health problems caused by chemical pollution, especially high-risk chemical pollution, have become a major factor affecting the public health. How to ensure that chemicals bring well-being to human society while ensuring the minimum harm to the environment and human health is a problem that needs to be solved urgently in the field of chemistry, especially environmental chemistry. This article summarizes the latest research progress in the risk identification, risk prevention, alternative research and development, and evaluation of perfluorinated compounds and other substances, and systematically explores how to use green chemistry, combined with the risk management and control, to decrease the risk of the high-risk chemicals during their entire life cycle. The article also discusses the research progress, development direction, and future development of high-risk chemicals throughout the life cycle. **DOI:** 10.16418/j.issn.1000-3045.20200924001-en

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Chemicals have caused environmental and health problems while bringing well-being to human society. In the beginning, the main concerns about the hazards of chemicals included explosions and acute toxicity during production, processing, storage, transportation, and use, and public hazards due to large-scale leaks. With the advancement of science and technology and the improvement of people's safety awareness, the environmental load and the persistence, bioaccumulation, and potential toxicity (PBT) risks of chemicals have attracted great attention. In response to the global environmental problems of toxic and hazardous chemicals, the international community and the governments of various countries have developed a series of international conventions on toxic and hazardous chemicals and priority risk management policies and regulations to restrict the production and use of specific chemicals. The alternatives for restricted chemicals have then been developed and extensively used to meet the demand for industrial development. However, the decoupling of synthesis with risk assessment makes some alternatives to be produced have potential risks as new environmental pollutants. Chemical pollution → alternative production → re-pollution has become a serious challenge in environmental chemistry.

How to ensure that chemicals bring well-being to human society while ensuring the minimum harm to the environment and human health is a problem that needs to be solved urgently in the field of environmental chemistry. Such challenges hasten the emergence of green development of chemicals. The green development of chemicals emphasizes the risk analysis as well as pollution warning and control throughout the whole cycle from the production, storage, transportation, use, discharge, and disposal of chemicals, which can achieve the prevention and control of pollution from the source.

1 Green development and risk prevention of chemicals

1.1 Overview of chemicals and their environmental health risks

Chemicals refer to the chemical substances with industrial and commercial properties produced through artificial purification, chemical reaction, and mixing. Due to the inherent physical, chemical, and biological reactivity (such as flammability, chemical stability, and insecticidal properties), chemicals have been extensively used in agriculture, industry, and social life, bringing well-being to the social and economic development. Currently, there are more than 164 million chemicals in the global market, and at least 10 million newly developed ones are launched on market every year. Chemicals have become indispensable materials and commodities for clothing, food, shelter, and transportation, with continuous growth in their production and consumption.

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However, chemicals affect and harm the society and environment while meeting the needs of human production and life. Since the 1960s, studies have proved the presence of synthesized toxic chemicals such as DDT in the Antarctic and Arctic regions. Such chemicals have PBT risks. Their residues can remain in the natural environment for decades and be accumulated and amplified in animals and humans through the food chain in a long term. With the improvement of research and detection, more and more synthesized toxic chemicals including pesticides, plastics, detergents, and flame retardants have been detected in the environment, which can cause endocrine disorders in fish, birds, and mammals, affecting the reproduction and development of organisms and even humans. Exposure to these chemicals in ultra-trace doses can cause biological aberrations, posing severe harm to the ecosystem and human health. Bisphenol A (BPA), a typical pollutant highly concerned by environmental scientists, is a high-yield chemical widely added to plastics and epoxy resin products. It is commonly found in a variety of environmental media such as air, water, and soil and can enter the human body through drinking water, air dust inhalation, and skin contact, causing severe health hazards [1]. Biological experiments have verified that BPA is endocrine-disrupting [2], which can cause adverse effects on the reproductive system and embryonic development of animals and increase the risk of breast cancer [3]. Epidemiological investigation shows that the cumulative exposure of BPA has a significantly positive correlation with the incidence of prostate cancer. Besides, BPA exposure can lead to decreased sperm count and motility in mice [4]. Perfluorinated compounds (PFASs), another type of typical environmental persistent pollutants, are organic compounds with alkyl chain as the skeleton and hydrogen atoms partially or completely replaced by fluorine atoms. With low surface tension, low viscosity, and hydro-oleophobicity, PFASs are extensively used in chemical industry, fire protection, construction, machinery, aerospace and other fields. However, the high-energy C-F bonds in the molecules of PFASs make their properties stable and difficult to be hydrolyzed, photolyzed, and biodegraded, hence leading to their persistent existence in the environment. PFASs have been detected in different environmental media on a global scale, even in remote areas such as the seas and the "three poles" of the earth, indicating that they have become global pollutants and caused severe environmental problems [5]. Among them, the typical compound is perfluorooctane sulfonate (PFOS), which can be detected in different organisms and even humans. It features a long half-life, difficulty to metabolize, biological amplification effect, and significantly increased concentration with the increase in trophic level in the food chain [6]. Moreover, toxicological studies have proved that PFASs can cause a series of toxic effects such as liver toxicity, reproductive and developmental toxicity, neurotoxicity, and immunotoxicity, and have certain associations with human health problems [7,8]. The exposure of these chemicals to human and ecology are long-term, concealed, and lagging, which have constituted a public health risk and environmental safety crisis. Hence, it is crucial to strengthen the environmental management of chemicals and reduce their risks to the ecosystem and health from the source.

1.2 Chemical control and potential risks of alternatives

Toxic and hazardous chemicals are a global environmental concern with serious impact. Their management and control have become a consensus and challenge facing the international community. Governments of various countries have formulated a series of international conventions on toxic and hazardous chemicals and priority risk management policies and regulations. The European Union promulgated relevant legal provisions prohibiting the addition of BPA to infant-feeding bottles in 2011; its member states also strictly restricted the application scope of BPA and banned the use of BPA in a variety of food packaging materials successively [9]. In 2000, 3M, the world's largest producer of PFASs, cooperated with the United States Environmental Protection Agency (EPA) in stopping the production of PFOS and its derivates. In 2009, the Stockholm Convention on Persistent Organic Pollutants (hereinafter referred to as the Stockholm Convention) formally listed PFOS and its salts as new persistent organic pollutants and agreed to reduce and ultimately ban the use of such substances [10]. In 2016, the United States Food and Drug Administration (FDA) stipulated that three products containing PFOS and its analogs shall no longer be used as food contact materials (FCM).

Multiple alternatives have been developed and extensively used in many industrial fields to avoid the utilization restrictions due to the ban on some chemicals such as BPA and PFOS. However, instead of solving environmental problems caused by BPA and PFOS, these alternatives have induced new and even severer environmental problems. (1) The levels of alternatives in environmental media and even organisms have shown a rapid upward trend. (2) As the alternatives have similar structures compared with the banned parent compounds, they often have similar toxic effects.

Currently, BPA alternatives, as additives for different purposes, are widely detected in various environmental media. In particular, their concentrations in indoor dust, sediment, rivers, and soil are similar to or even higher than that of BPA [11,12]. Most of the alternatives have similar physical and chemical properties compared with BPA. For example, the water solubility of phenol structure can make them easily enter the water body and cause new environmental pollution. The alternatives for PFOS are even more. According to incomplete statistics, there have been more than 3 000 products of PFASs on the market as of the end of 2018, as inferred by the Swedish Chemicals Agency. The 6:2 fluorotelomer sulfonic acid (6:2 FTSA) can replace PFOS as an additive for foam extinguishing agent. International fluorine chemical manufacturers such as 3M, Asahi, and Solvay have submitted over 50 potential alternatives for PFOS. However, most PFOS alternatives still retain the toxic effects similar to PFOS and have been detected in multiple environmental media [13,14].

2 National conditions of chemical production and green chemistry in China

2.1 Excessive control does more harm than good

Facing the increasing synthesized chemicals and their severe environmental hazards and health risks, western countries have strengthened the control of chemicals and even proposed across-the-board control of PFASs as a class of substances to avoid the environmental problems of chemical pollution → alternative → re-pollution caused by the development of alternatives with structures similar to the parents [15]. However, we believe this is an overcorrection, especially for large developing countries like China. The across-the-board control measures on PFASs to reduce environmental risks once and for all can come at incalculable cost. (1) We have to admit that the excellent properties of some chemicals determine their irreplaceability in many fields. The special chemical inertness, hydro-oleophobicity, and surface activity of the C-F bond in PFASs determine the performance advantages of their products. If chemicals such as PFASs are subjected to across-the-board control and replaced with chemicals that do not contain C-F bonds, the products may have compromised performance and even fail to function in some application areas. (2) As the chemical production chain is continuous, the destruction of downstream industries will affect upstream applications indirectly. For example, the production of PFASs end raw materials is supervised by the Stockholm Convention. Comprehensive restrictions on the production of these raw materials will increase the cost and even cause interrupted supply. (3) China should develop management and control plans based on the actual situation of its development, rather than directly adopting those in western countries. Due to the first-mover advantage of the industrial revolution, western developed countries have monopolized the market and patents of many alternatives and alternative technologies and transferred most of the chemical entities with high energy consumption and high pollution to developing countries like China.

2.2 Proposal and connotation of green chemistry

The current management and control of chemicals in China is caught in a dilemma of unbearable and non-negligible. The ever-increasing number of chemicals, low-dose long-term exposure, and mixed toxicity of chemicals have put forward higher requirements and become greater challenges to the environmental risk research methodology of chemicals. How to ensure that chemicals bring well-being to human society while ensuring the minimum harm to the environment and human health is a problem that needs to be solved urgently in the field of environmental chemistry. The available theories and methods in environmental chemistry cannot help to fully realize the environmental risk assessment of existing chemicals and even industrial reagents under priority control. This dilemma is particularly serious in the development of alternatives. The solving of this tough problem needs the full consideration of chemical production, storage, transportation, use and discharge. That is, the critical methods and technologies for the identification and classification of chemical risk sources as well as pollution early warning and reduction throughout the life cycle should be developed for the formulation of the management system specification and framework applicable to the conditions in China. At the same time, new methods and technologies are adopted in green chemistry to reduce the production and use of chemical products detrimental to human health and environment and develop products more friendly and compliant with the requirements of environmental protection. The control starting with the initial raw materials, reagents, catalysts, solvents, to the final products and by-products, different from the idea of post-pollution treatment, will prevent pollution from the source. The alleviation of toxicity and bioaccumulation of alternatives, optimization of product yield, elimination of waste, and reduction of energy consumption in the production mainly involve the development of new synthetic methods and routes, the screening of new chemical raw material, the optimization of reaction conditions, and the research and development of green products.

The issues involved in green development of chemicals not only are the challenging scientific problems in chemical disciplines such as environmental chemistry and organic chemistry but also will drive the development of related disciplines such as physics, materials science, geology, environmental toxicology, molecular biology, and informatics. Green chemistry has become the frontier of international chemical science and new interdisciplinary science with clear social needs and scientific goals. The goal of green chemistry is to make rational use of resources and energy to reduce production costs and achieve pollution control from the source in line with the guideline of sustainable economic development. It links traditional chemistry disciplines with coordinated development of resources and environment, emphasizing the ecological value requirement and practice of chemistry.

3 Measures for chemical control and green development

Developing alternatives and leveraging the advantages of industry–university–research (IUR) cooperation and multidisciplinary research are imminent needs in China. This is not only a major requirement for China to fulfill the Stockholm

Convention but also an important task proposed in the National Implementation Plan for the Stockholm Convention on Persistent Organic Pollutants of the People's Republic of China. In the development of alternatives and alternative technologies, we should consider not only economic feasibility and use efficacy but also environmental acceptability and safety for producers, users, and consumers. Enhancing support for alternatives and alternative technologies will provide another opportunity to adjust the industrial structure, promote cleaner production, develop a circular economy, and build an environmentally friendly society in China.

On the basis of the fully understanding of the risks of existing chemicals, we should control the risks from the source of production while paying attention to and reducing the potential risks during use and disposal, to achieve the reduction and control of risks throughout the life cycle of such compounds. Only by combining risk awareness and life cycle management can the management of high-risk chemicals be effectively implemented. It is not only a crucial link to ensure ecological safety and population health but also a national demand for breaking through the green trade barriers of developed countries and developing the economy. The basic scientific problems of chemistry in the environment and green development involve the identification of chemical pollutants, environmental remediation, source control, evaluation of toxicity, environment and health, and development of circular economy. These issues are the frontiers in physics, chemistry, chemical engineering, mathematics, informatics, materials, biology, and medicine. Here we put forward four suggestions for the high-risk chemical control and green development.

(1) Rapid identification of pollution and early warning of ecological/environmental risks. For the rapid identification and risk warning of pollutants, it is necessary to develop high-throughput, rapid identification, and source analysis method for pollutants in the environment, green pollution control and solid waste recycling technologies, analysis methods for life-cycle environmental risk of high-risk chemicals, and screening technologies for environmentally friendly alternatives. Efforts should be made to develop technologies for chemical design, preparation, use, environmental safety evaluation, and distributed storage, identification, and encryption of information on the basis of available studies, as well as toxicological prediction of chemicals on the basis of structural dependence, omics, biological pathways, etc. The identification of key toxic components leading to typical environmental pollution facilitates the revealing of their environmental transformation mechanism, the tracing of their sources, and assessment of population exposure assessment. Biomarkers should be used to clarify the disturbance of pollutants on key signaling pathways, explain the toxic effect mechanism of regional key pollutants. On the basis of revealing the mechanism of possible body damage induced by regional pollution, rational proposals can be generated on emission reduction, treatment, and health risk blocking, and then technical support can be provided.

(2) Life-cycle analysis and risk assessment of chemicals. At the macro-level, research on the global long-distance cross-border transfer of pollutants needs to be carried out. At the micro-level, key technologies for in-situ characterization of environmental micro-interface should be developed for continuous observation of micro-interface structure, free-radical chain reactions, and transient state of intermediates, which will facilitate the research on the micro-distribution behavior and molecular mechanism of typical pollutants in different interface processes and the revealing of the key physical-chemical factors affecting the retention of pollutants in multiple environmental media. In addition, the mechanisms of the biological, microbial, photochemical, and valence state transformation and metal methylation of pollutants in different media should be studied to clarify the transfer and transformation mechanisms throughout the life cycle and the ultimate fates of pollutants. The research on the distribution behaviors and rules of chemicals in different media throughout the life cycle, as well as the risk source identification, classification, and sorting methods suitable for the confidence requirements of different disciplines should be supported. Efforts should be made to manage and control the risks of chemicals throughout the life cycle of production, use, and disposal. Meanwhile, the government should pay attention to the risk management of chemicals. It is necessary to learn from the mature and complete laws, regulations, and policies of developed countries in management and control and establish a set of risk assessment protocols suitable for the conditions in China.

(3) Development of green chemicals based on artificial intelligence (AI) and big data. Faced with the increasingly severe challenges of alternatives, we should develop high-throughput in vitro toxicity test techniques as well as predictive and translational toxicological methods. The standardization of test procedures and methods, the conversion of in vitro test results to in vivo toxicity endpoints, the systematic toxicological evaluation combined with multi-omics technologies, and the omics evaluation of combined pollution necessitate special attention. It is essential to develop large-scale chemical toxicity test and prioritized screening systems combined with AI and automation technology to improve the management and risk prevention and control of chemicals. The combination with AI technologies such as cloud computing, blockchain, and deep learning is expected to foster the technological development and theoretical upgrade of pollution prevention and control and risk warning. Moreover, the AI-based deep learning system can give a green chemical synthesis scheme starting from the structural design and theoretically evaluate the persistence, toxic targets, toxic effects, and health hazards of the alternatives. In this way, the synthesis, production, and discharge of potentially hazardous alternatives to the environment and organisms can be reduced from the source, and virtual

screening can be provided for the safe design of environmentally friendly alternatives.

(4) Acceleration and strengthening of the construction of a legislation system for the environmental management of chemicals. China has been a power in global chemical production and consumption. International management concept and legislation on chemicals have gradually transitioned from hazard management to risk management. However, China still implements the hazardous management for chemicals, with the formulation of Regulations on the Safety Management of Hazardous Chemicals and Measures for the Environmental Management Registration of New Chemical Substances, which, however, are far from meeting the actual needs for environmental management of chemicals. It is recommended that the legislation for the risk management of chemicals should be improved at the national level. The basic research and system construction of chemical risk assessment, as well as the construction and certification of laboratories for environmental pollutant analysis and the environmental laboratories with good laboratory practice (GLP) should be promoted. It is essential to establish a risk management and control coordination mechanism to enhance the cooperation between departments. With the active participation and independent management of enterprises, a chemical pollution liability insurance system can be established. The information disclosure and the public awareness of environmental management of chemicals should be supported for the construction of a chemical management system with national participation to ultimately reduce environmental damage and population health risks caused by chemicals.

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