COMPARISON OF THE BASIC PRINCIPLES OF GREEN AND SUSTAINABLE CHEMISTRY CONCEPTS AND THEIR IMPLEMENTATION IN THE QSAR METHODOLOGY

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The growth of global production and use of chemical products increases the risks associated with the adverse effects of hazardous chemicals on human health and the environment. In international practice, there is a shift in emphasis in regulating the circulation of chemical products. The use of administrative methods that require state-level control of the circulation of chemical substances, their mixtures and products derived from them is supplemented by methods to prevent the release of hazardous chemical products onto the market. The scientific direction of "green chemistry" aims to prevent the negative impact of chemicals on the environment and human health at the initial stages of chemical processes by reducing or completely eliminating the use of hazardous chemicals or improving the synthesis processes that produce thesechemical substances. "Sustainable chemistry" is a scientific concept that aims to increase the efficiency of the use of natural resources to meet human needs for chemical products and services. Sustainable chemistry includes the development, production and use of effective, efficient, more environmentally friendly chemical products and processes. The principles of sustainable chemistry take into account the use of the best available technologies, increasing the life cycle of chemicals used in technological processes, and increasing resource and energy efficiency in order to achieve sustainable development. The application of the basic approaches and principles of both concepts in the formation and development of chemistry, chemical technologies and other industries is the driving force of sustainable industrial development.

Keywords: green chemistry, sustainable chemistry, chemicals, safe handling, sustainable development

DOI: 10.24263/EDSD-2025-7-15
Received 15.05.2025
Received in revised form 19.09.2025
Accepted 06.10.2025

Introduction

With the growth of global production and use of chemical products, the risks associated with the adverse effects of hazardous chemicals on human health and the environment are increasing. Scientists Kalyan Kumar Rana and Suparna Rana give a number of examples of important environmental problems associated with the use or release of unsafe chemicals. «Environmental problems such as biomagnification of DDT, ozone layer depletion, the Cuyahoga River calamity (caught fire in 1969, mobilized the nation, made basis for passage of the US Clean Water Act in 1972), the Love Canal tragedy (neighborhood of Niagara Falls, New York, used to conceal over 21,000 tons of toxic wastes in 1950's by the then Hooker Chemical Company, caused a public health disaster and an urban planning disgrace in 1978), the Bhopal disaster (world's worst industrial disaster, occurred on the night of 2-3 December 1984 at the Union Carbide India Limited pesticide plant, almost 20,000 people died), the Chernobyl disaster (catastrophic nuclear explosion occurred on 26 April 1986 at the Chernobyl Nuclear Power Plant, Ukraine, USSR) and the latest Fukushima Nuclear Power Plant tragedy (meltdown of three of the plant's six nuclear reactors, when hit by the tsunami triggered by the Tōhoku earthquake on 11 March 2011) are all too familiar examples of chemistry gone wrong» (Rana & Rana, 2014). The implementation and application of key international approaches in the field of sustainable industrial development and green technologies in national systems for regulating the safe handling of chemical products plays an important role both in reducing the negative impact of hazardous chemicals and products containing them on the environment and human health, and in increasing the competitiveness of manufactured chemical products in international markets, as well as their attractiveness for industrial and household consumers in the domestic market (Zuin et al., 2021).

In international practice, there is a shift in emphasis in regulating the circulation of chemical products: from administrative methods that require the state to control the circulation of chemical substances and their mixtures released on the market, as well as to detect, destroy or neutralize harmful chemical substances formed as a result of chemical processes, towards preventing the release of hazardous chemical products onto the market using preventive measures based on the application of the principles of green and sustainable chemistry, best available technologies aimed at the sustainable development of industry in the long term (Karagölge & Gür, 2016). The purpose of this study is to compare the approaches of the two concepts - green and sustainable chemistry in this context.

The approach to stimulating and supporting scientific developments to create safe analogues of hazardous chemicals with a longer life cycle was enshrined back in 1992 at the UN Conference on the Environment in Rio de Janeiro in the relevant Declaration in response to the challenges associated with the industrial production of chemicals. Today, the development of global political commitments to review approaches to the production and use of chemicals in order to minimize the consequences of their negative impact on the environment and human health is taking place within the framework of the Strategic Approach to International Chemicals Management (SAICM) forum, established in 2006 with the United Nations Environment Program (UNEP).

The principles of green chemistry from the first years of SAICM's existence formed the foundation for the formation of approaches to the rational regulation of the circulation of chemicals and products containing them. Later in 2014, the UN Environment Assembly at its first session recognized a new term - sustainable chemistry, noting that the development and application of appropriate approaches to the regulation of the circulation of chemical products should primarily be of interest to enterprises of the chemical complex, since they bear special responsibility for the development, production and use of products containing them.

Green Chemistry: Starting Points

The scientific direction of "green chemistry" aims to prevent the negative impact of chemicals on the environment and human health at the initial stages of chemical processes by reducing or completely eliminating the use of hazardous chemicals or processes that produce these substances. As noted in his works by P.T. Anastas, any developments in accordance with the principles of green chemistry require innovative (innovative) approaches to the molecular design of chemicals, taking into account the statement that the danger of a chemical is a disadvantage of its molecular structure, and can be eliminated at the design stage: «Intrinsic hazard of a chemical substance or a chemical process can be designed to be minimized at every level of a process, whether it is toxicity, physical hazards (e.g., explosion, flammability) or global hazards such as stratospheric ozone depletion. Risks based on these hazards may rise from the nature of the feedstock and raw materials that are used in the chemical transformations as well as the final products that are made. Careful design will reduce or eliminate intrinsic hazards within chemicals and processes» (Anastas & Eghbali, 2010).

The concept of green chemistry is more limited to chemicals, products containing them, chemical processes and their technical feasibility and is based on 12 principles focused on chemical synthesis (Anastas & Warner, 1998):

1. Waste prevention: chemical synthesis should contribute to the prevention of waste generation with the aim of their subsequent neutralization or utilization.

2. Maximum atom economy: chemical synthesis should contribute to the maximum content of starting materials in the final product.

3. Hazard reduction: chemical synthesis should contribute to the production of chemicals with minimal toxicity (or its absence) for the environment and human health.

4. Creation of safer chemicals and chemical products: the chemical products created should be less toxic or safe, and correspond as much as possible to their functional purpose (qualitative characteristics).

5. Use of less hazardous reagents and reaction conditions: the use of any reagents should be minimized or completely eliminated, if it is necessary to use reagents, safer analogues should be used.

6. Increasing energy efficiency: whenever possible, chemical synthesis should be carried out at room temperature and normal pressure.

7. Use of renewable raw materials: Renewable resources (including secondary ones) should be used as starting materials, rather than resources from natural sources that are depleting, such as oil, natural gas, coal and other minerals.

8. Reduction of intermediate stages and processes of chemical production: Whenever possible, eliminate intermediate reaction stages and the formation of intermediate products in chemical synthesis in order to eliminate the need for additional reagents and the formation of additional waste.

9. Use of catalysts instead of reagents: Catalysis in chemical synthesis allows to reduce the formation of waste due to its efficiency, the possibility of multiple use of catalysts in the same chemical reaction, reducing consumption or completely eliminating reagents from chemical processes.

10. The desire to create degradable chemicals and chemical products: it is necessary to produce such products that decompose after use to form safe chemicals, without accumulating in environmental objects.

11. Real-time analysis to prevent the formation of pollutants: the inclusion of real-time monitoring and control in the chemical synthesis process helps to minimize or eliminate the formation of by-products (wastes).

12. Minimization of the risk of accidents: when producing chemical products (including the choice of their aggregate state), it is necessary to take into account the risks of accidents and emergencies, such as fires, explosions, unauthorized emissions into the environment, to minimize the likelihood of their occurrence.

The application of the concept of green chemistry has been largely reflected in the activities of the US Environmental Protection Agency (EPA). It generally indicated the positive impact of the application of green chemistry principles on the development of a sequence of steps to prevent environmental pollution, in particular by eliminating or reducing sources of chemical hazards (Clark, 1999). Specific measures that allow reducing the negative impact from the source of pollution include appropriate modifications and changes in equipment, production technology, technological processes and procedures, replacement of raw materials (for example, the use of secondary resources), changing the composition of final products or molecular design of manufactured chemicals, improving procedures related to equipment maintenance and inventory control. So, "Green chemistry is about reducing waste, raw materials, risks, energy, environmental impact and cost" (Ivanković, Dronjić, Bevanda & Talić, 2017).

The sequence of steps for applying the principles of green chemistry in practice is as follows (Li & Anastas, 2012):

1. Source reduction and prevention of chemical hazards, including:

• development of chemical products that are less hazardous to human health and the environment;

• production of chemical products using raw materials, reagents and solvents that are less hazardous to human health and the environment;

• design of chemical synthesis and other processes with a reduction in the formation of chemical waste or its complete elimination;

• design of chemical synthesis and other processes that consume less energy or water (natural resources);

• use of renewable raw materials or secondary resources obtained by processing waste;

• development of chemical products with the possibility of their reuse or recycling;

• reuse or recycling of chemical products.

2. Decontamination of chemical products in order to reduce their hazard before further disposal.

3. Safe disposal of non-decontaminated chemical products, but only if other options (use as a secondary resource) are impractical.

Green and sustainable chemistry

The term “sustainable chemistry” was proposed by the Environmental Chemistry Department of the German Chemical Society in the early 1990s. It is a broader concept than “green chemistry” in terms of balancing the needs of society in the present and the need to protect the environment in the future and focuses mainly on the life cycle of chemicals and products containing them, rather than on chemical synthesis. Sustainable chemistry is a scientific concept that aims to increase the efficiency of the use of natural resources to meet human needs for chemical products and services. Sustainable chemistry includes the development, production and use of effective, efficient, more environmentally friendly chemical products and processes. «The Concept of Sustainable Chemistry can help all actors to identify feasible technical alternatives in synthesis and production with less hazardous chemicals by taking into account sustainability criteria in areas beyond the scope of sound management of chemicals, like for instance resource and energy efficiency, the use of renewable feedstock, working conditions and the impact on communities of the production of chemicals» (Blum et al., 2017). Thus, this approach takes into account the environmental, economic and social aspects of industrial development.

The main principles aimed at a more integrated approach to the management of chemicals and natural resources are established by Directive 2010/75/EU of the European Parliament and of the Council on industrial emissions (integrated pollution prevention and control). These principles take into account the use of best available technologies, increasing the life cycle of chemicals used in technological processes, increasing resource and energy efficiency in order to achieve sustainable development, i.e. a balance between human activity and socio-economic development - on the one hand, and natural resources and the ability to restore the natural environment - on the other hand (Kümmerer, 2017). There are different approaches to the implementation of sustainable chemistry, but the main technical directions that were identified in 1999 largely coincide with the approaches used within the framework of green chemistry (Collins, 2001):

1. Qualitative development: use of safe chemicals or, if this is not possible, chemicals with a low risk of negative impact on human health and the environment, resource-efficient production of products with a long service life.

2. Quantitative development: reduction of consumption of natural resources, which, if possible, should be renewable, as well as prevention or minimization of emissions and intentional release of chemical (including polluting) substances into the environment. These measures allow to reduce production costs.

3. Comprehensive assessment of the life cycle of products: analysis of the production of raw materials, as well as the production, processing, use and disposal of chemicals and substandard chemical products in order to achieve resource and energy efficiency, prevent the use of hazardous chemicals.

4. Action instead of reaction: preventing the release of chemicals that pose a risk to human health and the environment throughout their life cycle, including chemicals that exert a significant burden on ecological systems (for example, persistent organic pollutants) at the stage of their development; reducing the cost of damage and associated economic risks for industrial enterprises, as well as possible costs of restoring the natural environment at the expense of the state.

5. Economic innovations: "resistant" chemicals, chemical products and methods of their production inspire confidence in both industrial and household consumers, as well as the public sector, which in turn provides competitive advantages for these products.

As can be seen from the description above, the main approaches used within the framework of the concept of sustainable chemistry largely reflect the principles of green chemistry, but have a broader scope. For greater clarity, the main characteristics of the two concepts are presented in Table 1.

However, none of the concepts described above, despite their importance for the sustainable development of industry, can and should not replace the need for rational regulation of the safe handling of chemicals and chemical products containing them at the legislative level (Schulte, et al., 2013).

The application of the principles of green and sustainable chemistry as reinforcing and complementary components, as well as the emphasis on the life cycle of chemicals or processes in the formation and development of the chemical regulation system, not only promotes innovation, but also reduces the risk of associated problems (for example, to prevent the use of toxic reagents for wastewater treatment, the production of which has the greatest negative impact on the environment than untreated wastewater, to prevent the production of chemical products with improved consumer properties, which are classified as highly toxic to humans or persistent in the environment, to avoid the use of such technologies, which result in the formation of hundreds and thousands of units of waste per unit of final product, etc. The main principle, common to the two analyzed concepts - the creation of safer chemicals and chemical products, is reflected in the recommendation to replace hazardous chemicals with chemicals that are classified as lower hazard classes or, if possible, not classified as dangerous.

Table 1 – Key characteristics of green and sustainable chemistry concepts

Characteristic	Green chemistry	Sustainable chemistry
Prerequisite	US Pollution Prevention Act, 1990.	EU Directive 96/61/EC concerning integrated pollution prevention and control, 1996
Definition	An approach to chemical synthesis that involves reducing or eliminating the use of hazardous chemicals or processes that generate hazardous substances to reduce negative impacts on the environment and human health	A scientific concept aimed at increasing the efficiency of natural resource use to meet people's needs for chemical products and services (development, production and use of effective, environmentally friendly chemical products and processes)
Scope	1. The creation and use of chemicals and processes that are practically non-polluting to the environment. 2. The approach is limited to chemicals, products, processes and their chemical synthesis.	1. Supporting environmentally sound development, i.e. a balance between meeting the needs of society today and protecting the environment for future generations. 2. A broader approach to taking into account economic and social aspects.

QSAR methodology in the development of the concept of sustainable chemistry

At the same time, the problem of finding accessible and fast methods for identifying the properties of unstudied chemicals has always been relevant for both representatives of the chemical industry and the regulator, including supervisory authorities. In order to reduce the burden on industrial enterprises associated with the need to conduct laboratory tests to obtain the necessary information about the properties of new chemicals, further assess their danger and potential risks to human health and the environment, it is recommended to use data obtained by alternative methods, including by predicting hazard indicators using the QSAR (Quantitative Structure-Activity Relationship) methodology (Gbadago et al., 2024). This approach, based on mathematical moderation and mathematical statistics methods, allows the structures of chemicals to predict their properties without conducting laboratory tests. For example, the QSAR Toolbox software, developed to eliminate gaps in information on the toxicity and ecotoxicity of chemicals by the European Chemicals Agency, makes it possible to group chemicals into toxicologically significant categories, find safer analogues for them, and predict their properties both on a qualitative basis levels (including determining the potential for negative effects of a chemical substance on a living organism with a particular route of entry), and at the quantitative level, including predicting numerical values of specific toxicological and ecotoxicological indicators (Singh et al., 2024).

Today, the QSAR methodology is recognized as a successful international practice and is used in many scientific and research developments in the field of chemistry, biology, toxicology, and pharmacy in order to predict and further classify the physicochemical, toxicological, and biological activity of new chemical compounds being developed or synthesized. First of all, this tool plays a crucial role in the field of pharmaceutical developments in identifying promising directions for designing drugs even before they are launched into industrial production. The widespread use of QSAR mathematical modeling allows not only to significantly reduce and, in some cases, completely eliminate the need for expensive laboratory research and experiments related to the development of fundamentally new chemical compounds, but also to predict such properties of the created chemical substances that would reduce their negative impact on the environment and human health while maintaining quality characteristics that meet the needs of the potential consumer.

Authors Gramatica P., Papa E., & Sangion A. have presented some examples of how explorative analysis by PCA combined to QSAR modeling can be useful to screen, rank and predict complex behavior of chemicals in the environment. «QSAR models generated for the cumulative indexes, which are derived from the combination of multiple endpoints, link these new macro-endpoints to the potential hazard inherent in the chemical structure and can be proposed for preliminary priority setting purposes both for compounds without experimental data and for new chemicals». This approach is helpful to avoid the synthesis, the commercialization and the release in the environment of harmful compounds, which would be recognized as dangerous only after evidence of human health concerns was manifested. This is the basis of the "benign by design" approach of Green Chemistry (Gramatica, Papa, & Sangion, 2018).

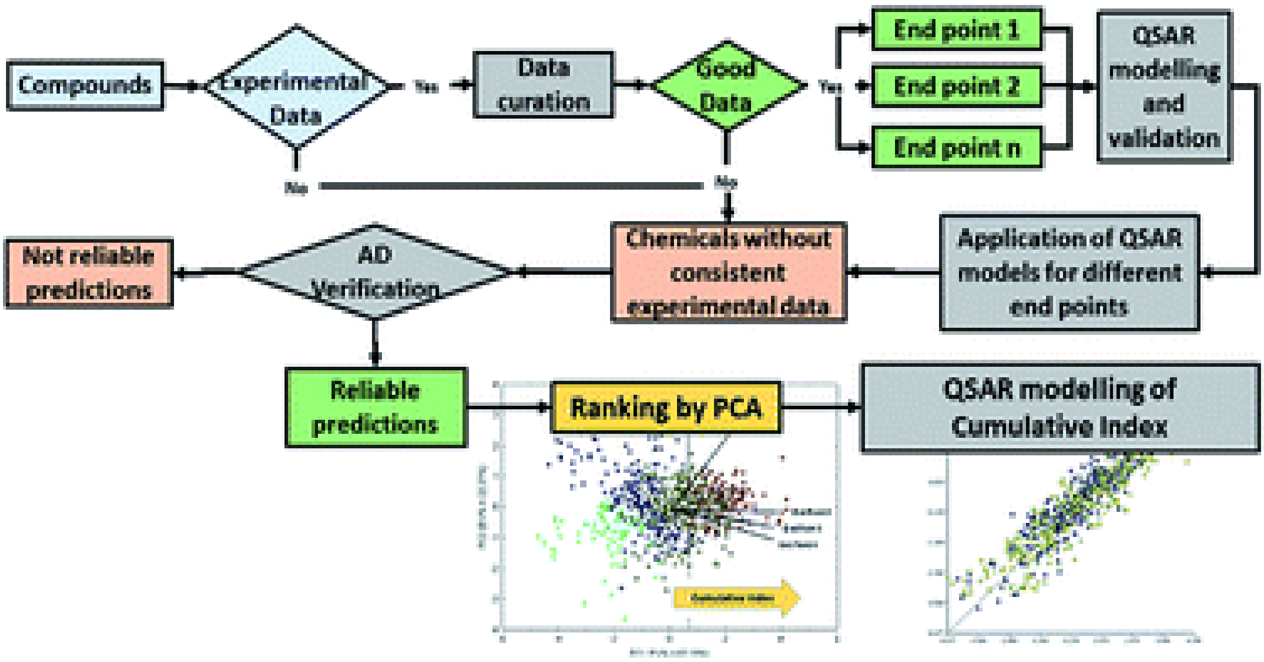

Figure 1. Conceptual scheme of the QSAR modelling of PCA end-points (Gramatica, Papa, & Sangion, 2018)

Conclusions

Approaches that utilize green chemistry principles are needed if all the nations are going to meet their societies' needs without compromising the ability of future generations to meet their own needs.

The application of the basic approaches and principles of two concepts - green and sustainable chemistry - in the formation and development of the technical system, including with the aim of gradually eliminating from circulation chemicals that have the most serious consequences for the health of the population of current and future generations, and replacing them with safer analogues, is certainly a driver for the sustainable development of the industry.

In coming days, expansion of green chemistry needs to increase at an accelerated pace if molecular science is to meet challenges of sustainability. We need the relevant scientific, engineering educational and other communities to work together for sustainable future through green and sustainable chemistry.

To achieve such sustainable chemistry requires a sea change in the chemical community. The principles of green or sustainable chemistry must become an integral part of chemical education and practice.

Conflict of interest

The authors state no conflict of interest.

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