Reaching Circular Economy through Circular Chemistry: The Basis for Sustainable Development

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Circular chemistry (CC) is an approach for establishing chemical processes to become truly circular and sustainable. It adopts the principles of circular economy (CE), employing life cycle approaches and systems thinking, which help to understand and address the sustainability issues of chemical processes and products. Within this whole context, it is possible to identify some problems of the current lifestyle, such as plastic waste disposal, CO2 emission, e-waste, among others, which need to be addressed accordingly. The reuse provided, well-structured within the context of circular chemistry, can bring benefits in all spheres: social, environmental and economic. Thus, the purpose of this revision is to present CE and CC as the pillars for a sustainable development, bringing discussions about: CE and CC systems; sustainable chemistry; and chemistry 4.0, which embeds digitization, sustainability, and circular economy in industrial chemical processes. Through the knowledge of chemistry, both CC and CE can contribute with innovative methods and processes which maximize benefits, eliminating, or, at least, reducing adverse impacts, thus contributing to construct a mutually beneficial relationship between science and society, its surroundings, and the environment. Therefore, implementing this new model is an opportunity that challenges the human imagination in building a better world.

Keywords: circular economy, circular chemistry, sustainable development, sustainability

1. Introduction

The challenge humanity has ahead is enormous. Across the planet, billions of people still live in extreme poverty,1 without access to clean water or food in minimally sufficient quantities; millions die each year from diseases transmitted by viruses, bacteria, protozoa, helminths, and fungi; climate change has accelerated the desertification of previously habitable areas while the rising of the oceans’ levels threatens to make entire archipelagos disappear; millions of people are forced to leave their homes and cities by wars and conflicts, in one of the largest waves of migration that has been reported; unemployment, especially among young people, is increasing, especially in countries where production processes have become more automated and less dependent on human labor; the intense exploitation
of the planet’s natural resources and the generation of large amounts of waste have severely affected the quality of air, soil, and water bodies.

According to the United Nations Environment Program (UNEP), cities worldwide will produce around 2.2 billion tons of waste every year up to 2025, which will be more than three times the amount produced in 2009. The consumption of minerals has increased exponentially, and further growth is expected until at least 2050. In order to meet this increasing demand, more metals will have to be produced, raising questions about sustainability. In addition, the mineral industry causes significant environmental problems. The production of non-metals represents about 7% of global carbon dioxide (CO₂) emissions. Among the options for mitigating this problem, carbon capture systems stand out, but they are not yet ready for commercialization.

Metals such as copper, aluminum, iron, as well as noble or rare metals, are used in different industrial segments (e.g., construction, electronics, automotive, catalysts, energy, among others). Metals are extracted from natural deposits, often difficult to access, causing contamination and damage to soil and biodiversity, when not major disasters, such as those that occurred in Mariana/Brazil (2015) and Brumadinho/Brazil (2019). Furthermore, there are predictions that the material from recycling by itself will not account for the growing demand in the future.

Tens of thousands of industrial chemicals are created, produced, and marketed worldwide annually, generating waste that is now present in the most different types of environmental compartments. For instance, plastics, used for different applications, contain in their composition (in addition to one or more monomers) different types of additives-such as plasticizers, antioxidants, stabilizers, flame retardants, among others, posing different degrees of toxicity to living beings and becoming more challenging to separate.

Plastic pollution in aquatic ecosystems has grown sharply in recent years and is expected to more than double by 2030, with consequences for health, the global economy, biodiversity, and climate. Studies indicate that greenhouse gas emissions in 2015 from plastics were 1.7 Gt of CO₂ equivalent, and are expected to increase to approximately 6.5 Gt CO₂ equivalent by 2050, or 15% of the carbon budget.

Although they can be pointed out individually, these problems are interconnected, with solutions that depend less on specific actions and much more on unified approaches. In addition, the resulting effects can differ significantly in intensity, as economic and social inequalities are accentuated among nations.

In this sense, it is urgent to seek integrated solutions to add new knowledge and develop technologies, processes, and products capable of consuming fewer natural resources and energy, as well as minimize the generation of final waste. Furthermore, all those solutions need to be readily accessible to the entire population.

In Brazil, in recent decades, the country has made considerable advances in science and technology (S&T), with significant improvements in different areas, resulting, in many cases, in more sustainable products with higher added value. Just to name a few examples, research on Brazilian Agricultural Research Corporation (EMBRAPA) helped to make the country one of the largest agricultural powers on the planet, developing plant varieties more resistant to pests and climate change and with a higher productivity per cultivated area; as a global leader in the use of biofuels in its vehicle fleet, Brazil is today one of the world’s producers of second generation ethanol (2G ethanol), using sugarcane waste for its production; and the EMBRAER’s aircraft, sold in several countries around the world, were born from an initial development made in the Department of Aerospace Science and Technology (DCTA) of the Technological Institute of Aeronautics (ITA). Also recently, Brazilian researchers were the first to establish the correlation between the Zika virus and a form of microcephaly, with our research groups acting rapidly on the vaccine development.

It is worth noting that these advances were only achieved with significant public investments in universities and research centers - with contributions, in some instances, also of research carried out in private and public companies - which resulted in a significant increase in the formation of new professionals in the graduate level. Looking ahead, however, it looks necessary to expand the interaction between research institutions and the production chain, integrating new knowledge with innovation in products and processes, which could result in creating new niches and opportunities and adding value to the goods produced.

Furthermore, it is essential that all the resulting development should be aligned with an economically and socially fair and sustainable environment in a modern social market economy. Looking at this panorama, chemistry, as a central science and driver of innovation, can play an important central role in this process.

These days, the domains of circularity, sustainability, and resilience are essential for a prosperous society. In terms of sustainability, low carbon chemistry is taking on increasing importance, and therefore, link it to the concept of circular economy will play a vital role for bind the principles of green/sustainable chemistry more comprehensively in the resource-dependent chemical industry.
Bibliographic data were retrieved from the Web of Science database on February 16th, 2022, using the keyword “circular chemistry” (CC) and further analyzed with the VOSviewer software (version 1.6.17) aiming to identify trends in circular chemistry. Figure 1 shows the bibliometric map of co-occurrence and temporal trend of terms from the field of circular chemistry. It is possible to observe that the most dominant themes and most discussed by researchers are Green Chemistry, catalysis, management, polymers, and recycling. Figure 1 also shows that the latest research trends in circular chemistry are associated with sustainability, circular economy (CE), biomass, circularity, and bioeconomy. Therefore, this result suggests greater attention to these topics that are currently being researched and published. It is important to note that the terms with the yellow caption are the most recently discussed topics related to CC.

Thus, discussions which detail the drivers that enable circularity and the approach/methodological tools that help the practice of circularity in the chemical industry domain are of paramount importance. The authors will outline the contributions that chemistry has made to the implementation of a CE model and how this can be increased, as well as point out the main challenges that are posed for the future, on a global scale and in Brazil. In view of the above, this review article intends to present CE and CC as one of the possible paths for sustainable development, bringing concepts, themes, discussions, and directions for the circularity of the processes.

2. Circular Economy

In recent years, the world industry has been undergoing a profound transformation, shifting from a linear to a circular model due to economic, social, and mainly environmental developments. The linear economy is based in processes of extracting, producing, and disposing of waste. Resources are extracted from nature, transformed into consumer goods, and disposed of at the end of their ‘useful life’. In addition, over the lifecycle of a product, losses and waste occur.

The production of goods is today, mainly based on the linear concept of the economy, in which they are mostly produced from new resources extracted from nature and through conventional energy sources, while at the end of their lifecycle they are discarded into the environment. Or, at best, they may be partially recycled, only in relation to their most valuable components, generating a representative amount of waste.

The linear economy (Figure 2), based on “extraction-production-consumption-disposal,” impacts in two ways: (i) by removing natural resources from the environment (extraction of oil and gas, mining, unsustainable crops), and (ii) by the reduction in the intrinsic value of natural resources, caused by the disposal of waste and the consequent environmental pollution.

In considering those problems, there is a consensus today that this linear model must be replaced, on a comprehensive scale, by a new model, circular in its conception, able not to
cause negative impacts on the environment by a low waste production throughout processes and during the life cycle of the products, minimizing the disposal of pollutants into the environment.\(^{16}\)

This new paradigm can be defined as “a systemic approach to economic development designed to benefit businesses, society, and the environment” which “aims to gradually decouple growth from the consumption of finite resources.”\(^{17}\) A circular economy is “regenerative from the project and aims to keep products, components, and materials at their highest degree of utility and value for all the time.”\(^{17}\) This conception is based on three principles, applicable to all forms of production, namely: (i) eliminate the generation of waste and pollutants from the beginning of the process; (ii) keep products and materials in use; and (iii) recover systems impacted by nature.\(^{17}\) Added to that, the circular economy is also based on the 3Rs: reduce (a reduction in the use of raw materials and thus in environmental impact of production); reuse (through the extension of the life cycle of goods); and recycle (waste diversion).\(^{13}\)

The circular economy (Figure 3) prioritizes products, processes, and activities that valorize energy, materials, and labor, focusing on durability, reuse, recycling, and remanufacturing. Therefore, new discoveries, applications, and innovation must be coupled to this new way of producing, consuming, and using, where the exploitation of natural resources, the generation of waste in production, the use of non-renewable energies, and final disposal should be replaced by environmentally sustainable models.

In this panorama, chemistry emerges as a fundamental science being responsible for the development of new materials, the synthesis of new substances and, together with biology, the explanation of the mechanisms that regulate systems as complex as life. Thus, chemistry acts on basic and applied sciences and makes use of the results in developing processes and products through its industrial sector.

In the linear model of the economy, the impacts derived from different steps in the production chain, such as poor practices of use and disposal, associated or not with
properties which belong to certain classes of substances (e.g., persistence in the environment and/or toxicity for certain species), have caused some of the great problems faced by humanity in the 20th and 21st centuries. Undeniably, either directly or indirectly, chemistry is associated with several of them. Thus, pesticides, used to protect cereal crops and improve productivity per planted area, were synthesized to meet the demand for food from a globally increasing population. However, their use negatively affects beehives and their pollination cycle, which would also cause a drop in production. Another emblematic example is plastics, widely present in our daily life in most different applications, that are releasing their chemicals into rivers and oceans, threatening their fauna and flora species and, ultimately, entering the food chain.

On the other hand, the development of all branches of chemistry in the last eight decades - in which several advances have been made - has provided, for instance, the discovery of new drugs (such as new antibiotics, antivirals, and chemotherapy drugs, among others); new polymers to produce lighter and more resistant plastics for the most diverse applications; and the development of new alternative energy sources, renewable and with fewer impacts on the environment.

Chemistry, in its various fields of activity and expertise, can undoubtedly contribute significantly to the migration of the world economy from its current model to a more environmentally sustainable alternative by emerging from this new scenario either supporting other fields of science or boosting new emerging fields. Indeed, chemistry can play a relevant role in promoting the eradication of hunger, making megacities more inclusive and safer, and protecting and conserving the oceans, seas, and marine resources. In this sense, it is essential to envision some sectors where these changes may produce more significant and immediate impacts. It is worth mentioning food production and crop protection; the preservation of the quality of water resources; the reduction of greenhouse gas emissions; the development of new ways for clean energy production; and the development of new biodegradable polymers, among others.

It is noteworthy that chemistry, once acquiring the role of protagonist within this new model, should become the science and industry of reuse, integrating processes and chemically simplifying products in order to make them easily reversible to more simple and reusable materials, with lower consumption of energy and natural resources.

It is very likely that in the near future, chemistry will modify its current focus, which comprises the study and manipulation of atoms and molecules, to something closer to what atoms and molecules play in dynamic systems, and how they can be controlled and manipulated on an atomic and molecular scale. On the one hand, if this tends to bring considerable changes in the way of thinking and doing chemical science, technology and innovation (S,T&I), as well as of educating the new generations, the possibilities of openness to new fields of action seem endless. In addition to this question, in 2018, Guarieiro et al. presented the six chemistry mobilizing axes, highlighting the importance of aligning scientific and technological research, considering the central role of chemistry in solving problems and overcoming challenges affecting education, full citizenship, climate change, food production and quality, access to and quality of water, energy security, preservation of ecosystems and species, emerging diseases, and quality of life.

2.1. Innovative business models

The concepts of circular economy and circular chemistry have only recently begun to be discussed globally. As an important contribution to a sustainable future, chemistry must be adapted to a circular economy by eliminating waste, circulating and recycling products, and saving resources and the environment. The awareness of the finite nature of many resources and the limited environmental tolerance towards the chemical industry has grown enormously in the past years, making it somehow evident that linear production is not supported for much more time. It is not environmentally and economically affordable to keep consuming scarce resources with their value-added products to be decomposed and/or degraded to waste without considering reuse, recycling, upcycling, recovering, repurposing, and remanufacturing by maximizing atom circulation. Currently, governments and stakeholders are in a position to either decide or not in favor of more ambitious and urgent worldwide action toward sustainable development since “business as usual” is not an option anymore.

As the circular economy and sustainability gain greater attention from governments, industry, and academia, sustainability-oriented business model innovation is becoming fundamental, being an important source of sustainable competitive advantage among companies. In all objectives, it is clear the outstanding importance that S,T&I will have for its reach, especially when considering the time window established by the United Nations (UN).

In this sense, companies wishing to follow circular practices must adopt an innovative perspective that is not limited to a change in the supply chain but which considers the existence of multiple cycles of value creation to minimize the need to dispose of products at the end-of-life, thus ensuring the sustainability of the entire process.
The innovation of the sustainable business model aims to integrate sustainability aspects into its projects and implement sustainable business models.36

Geissdoerfer et al. conducted a comprehensive review of the sustainable business model innovation literature. Moreover, they identified various definitions and interpretations of the main concepts. The authors defined business model innovation as “the conceptualisation and implementation of new business models. This can comprise the development of entirely new business models, the diversification into additional business models, the acquisition of new business models, or the transformation from one business model to another”. And they came up with four innovative types of sustainable business models; (i) sustainable start-ups; (ii) sustainable business model transformation; (iii) sustainable business model diversification; and (iv) sustainable business model acquisition, as shown in Table 1.

| Type                              | Definition                                                                 |
|-----------------------------------|---------------------------------------------------------------------------|
| Sustainable start-ups             | a new organization with a sustainable business model is created            |
| Sustainable business model        | transformation                                                             |
| transformation                    | the current business model is changed, resulting in a sustainable business model |
| Sustainable business model        | diversification                                                           |
| diversification                   | without major changes in the existing business models of the organization, and additional sustainable business model is established |
| Sustainable business model        | acquisition                                                                |
| acquisition                       | an additional, sustainable business model is identified, acquired, and integrated into the organization |

Sinkovics et al. performed an umbrella review of 57 systematic literature reviews related to sustainable business model innovation, aiming to classify the guidelines of the sustainable business model. The main types of business models related to the concept of innovation in sustainable business models comprise (i) sustainable business model; (ii) base (bottom) of the pyramid business model; (iii) circular business model; (iv) lean and green business model; (v) product-service system; (vi) sharing economy business model; (vii) sharing economy business model; and (viii) integrative business model.

Sustainable business model innovation is a complex and multifaceted phenomenon, making it necessary to explore several aspects. Therefore, sustainable business models may have different guidelines depending on the goals and motivations driving the innovation process. Lastly, Mohan et al. highlight the need for and importance of innovation in sustainable business models for the future success of the bioeconomy.

Like the circular economy, there is no single universal definition of a bioeconomy. As this is an emerging field, there are different interpretations. However, it is perceptible that the bioeconomy is related to using renewable biological resources, such as biomass, to produce renewable biofuels, bioproducts, and biopower for economic, environmental, and social benefits. The economy has been an essential tool for achieving the goals of sustainable development.39

Sustainable bioeconomy proposes sustainable biomass feedstock production, biomass conversion processes, and products in addition to substituting fossil resources for renewable resources. Recently, around 50 countries worldwide have adopted national bioeconomy strategies as a path to more sustainable forms of production, especially concerning achieving the 17 Sustainable Development Goals (SDGs) of UN (details about the SDGs are presented in section 3). The purpose is to control the effects of climate change while providing a renewable source of carbon (biomass), thus favoring economic development. Moreover, a sustainable bioeconomy can be achieved by integrating with other interdisciplinary areas, such as the circular economy.

According to Schoenmakere et al., bioeconomy and circular chemistry converge on five different agendas, (i) economic, (ii) resources, (iii) environmental policy, (iv) social transition, and (v) research and innovation, as presented in Figure 4.

According to Leong et al. and Tan and Lamers, combining the bioeconomy and the circular economy generates a new concept known as the circular bioeconomy. Circular bioeconomy is based on the cascading use of biomass from biological resources in accordance with a systemic economic development approach. This concept focuses on the idea of recycling, reuse, remanufacture, and maintaining a sustainable manufacturing process, to generate useful bioproducts and promote a more sustainable structure.

The circular bioeconomy has gained prominence in terms of innovation with the development of new products and processes. The pillars for the development of the bioeconomy are technological innovation, regional development, and competence formation, as well as industrial collaboration.

3. Sustainable Chemistry

Sustainable chemistry is a recent development in the applied sciences. While the concept of Green Chemistry was formulated through the widely known 12 principles and has been applied since then in the concept of linear economy, sustainable chemistry has recently evolved as...
a closely related but more holistic concept.\textsuperscript{3,27} Although Green Chemistry has been a guideline for good practices in chemical companies and research laboratories around the world for the last 25 years, some parts of it may not be sustainable at all.\textsuperscript{47} While Green Chemistry is quite suitable for the optimization of linear production routes, the concept of sustainable chemistry has been discussed as being applied to circular chemistry processes.\textsuperscript{18,47} However, re-evaluating and re-adjusting chemistry towards a circular economy requires a consistent definition of a sustainable chemical process and needs to take into account people, planet, and profit level (the “triple bottom line”). Clearly, in order to innovate in chemistry towards sustainability to become feasible, it needs to have economically viable applications.\textsuperscript{18}

The understanding of sustainable chemistry has been subjected to different interpretations over the years. According to the OECD (Organization for Economic Co-operation and Development), sustainable chemistry is “a scientific concept that seeks to improve the efficiency with which natural resources are used to meet human needs for chemical products and services. Sustainable chemistry encompasses the design, manufacture, and use of efficient, effective, safe, and more environmentally benign chemical products and processes.”\textsuperscript{48} Some other definitions do not differentiate Green Chemistry from sustainable chemistry, such as those by the US Environmental Protection Agency, the American Chemical Society, the Royal Society of Chemistry, and International Union of Pure and Applied Chemistry (IUPAC).\textsuperscript{49-51} In turn, the Brazilian Chemical Society has initiated the discussion of sustainable chemistry through the “Movimento Química Pós 2022 - Sustentabilidade e Soberania” (which in direct translation to English, it means “Action of Chemistry post 2022 - Sustainability and Sovereignty”) towards the establishment of sustainable chemistry.\textsuperscript{52} Indeed, sustainable chemistry is in close agreement with circular chemistry (as critically discussed in section 4), in the way they are complementary to each other.

In order to meet sustainability,\textsuperscript{53-55} chemistry needs to be developed (and innovated) in a way that the whole lifecycle of chemical products is fully considered, and no materials should be wasted or lost in the production chain.\textsuperscript{56} Moreover, sustainable chemistry (Figure 5) includes system innovations, which, in turn, will fundamentally contribute to changes in the social (values, regulations, attitudes, among others) and technical (infrastructure, technology, tools, production processes, among others) dimensions and the interactions between them.\textsuperscript{56} Indeed, by contributing to and adopting sustainable chemistry practices, the chemical industry faces a unique opportunity to evolve and innovate. This will probably result in good economic advantages for the industry in the medium to long term.

Blum \textit{et al.}\textsuperscript{56} have proposed seven principles of sustainable chemistry (Figure 5). These principles are (i) design of benign chemicals, (ii) development and use of alternative solutions for problematic applications, (iii) reduction of impacts, (iv) conservation of natural resources, (v) promotion of reuse and recycling, (vi) increase of market and opportunities, and (vii) application of corporate social responsibility. Indeed, sustainable chemistry is completely inserted into the definitions of circular chemistry and circular economy.

Historically, the chemical and related industries have developed and supplied different S,T&T solutions for addressing many global challenges.\textsuperscript{57,58} Although the chemical industry has also helped to develop products and processes favoring environmental protection through pollution prevention and greenhouse abatement technologies, among others, those are still not enough to meet the goals of the 17 SDGs from the UN, the Agenda
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Therefore, the sustainability of the planet and the guarantee of delivering a habitable planet for the next generations have not yet been achieved. Nevertheless, the chemical industry and the field of chemistry have a unique role to play in achieving these goals.\(^5\)

Indeed, the chemical industries and related technologies are essential for human well-being and modern societies, with more than 95% of all manufactured goods and articles relying on chemistry.\(^8\) Within this context, while chemicals provide many desired benefits, they may be intentionally or unintentionally released during their lifecycle, possibly causing adverse effects on human health and the environment.\(^8,26,30\)

Nowadays, considering the study by Wang \textit{et al.},\(^8\) over 350,000 chemicals and mixtures of chemicals have been registered for production and use, up to three times as many as previously estimated,\(^7\) with substantial differences across countries and regions over the globe. Another finding from Wang \textit{et al.},\(^8\) is that the identities of many chemicals remain publicly unknown because they are claimed as confidential (over 50,000) or ambiguously described (up to 70,000). This situation puts humanity in some difficult dilemmas: How to develop lifecycle practices and recycling/reusing of those chemicals whose identities remain unknown? How could they be correctly and safely managed under these conditions? Of those, how many are hazardous and/or risky to human health and the environment? How to evaluate and develop good practices in manipulating them? How to promote the cycle of life studies with them? Those points are very challenging to be solved accordingly, since new chemicals are becoming more complex regarding their chemical structures (for instance, stereochemistry, (poly)functional groups, among others).\(^7\) Indeed, this kind of problem is yet to be solved. For that, the chemical companies and academia still need to develop solutions soon, with mutual benefits if they work synergistically.

Even though one of those chemicals is produced in one country or region, it may enter or be distributed to another country by trade (e.g., as imported goods) and/or through environmental transport (via the atmosphere, rivers, oceans, and soils). In this way, the circular economy and sustainable chemistry must be worked on globally; acting locally or regionally is important, but not sufficient. In order to manage chemicals within a country, it is necessary to address not only chemicals manufactured in, imported into, and/or used in the country but also those manufactured, used, disposed of, and released in other countries. The demand for chemistry to fit into this scenario is tremendous and very complex.\(^8,27\) In this way, a chemical produced in one place eventually pollutes transboundary regions, which could eventually lead to geopolitical misunderstandings among different countries or governments. Nonetheless, international cooperation is strongly suggested in addressing the challenges humanity faces in achieving a sustainable future.

Figure 5. Objectives and guiding Principles of Sustainable Chemistry (based on data from Blum \textit{et al.}).\(^5\)
On the other hand, the Earth is running out of resources needed for manufacturing commodities such as chemicals, minerals, and petroleum. In addition, these components are available only at ever-increasing economic and environmental costs. One of humankind’s greatest challenges over the 21st century is how to provide adequate resources for humanity. Most geological materials extracted so far have been converted into products and finally to waste (e.g., in the linear economy mostly employed until now). One such emblematic example is the current semiconductor shortage, which is required for microchip production, has disrupted the global supply chain and pushed down shortage, which is required for microchip production, has disrupted the global supply chain and pushed down shortfalls of relevant chemicals. And, depending on which present semiconductor shortage as well as future worldwide shortages of relevant chemicals. And, depending on which aspect of a particular problem is considered, urban mining of e-waste is becoming more cost-effective than virgin mining. According to a study from Zeng et al., this is already true for the elements copper and gold, which can be mined from e-waste and may be reutilized in a variety of applications in modern life.

Synthetic chemicals are considered to be ubiquitous in the human body and all environmental compartments. Since these chemicals are man-made, there hardly are natural routes for them to be efficiently degraded or decomposed. Consequently, synthetic chemicals are often persistent and bio accumulative in the environment, eventually making their way into the food chain. Ultimately, these chemicals, by participating in the food chain, may affect human health. Chemical pollution has become a major cause of disease and premature death, not only from occupational exposure in workplaces but also from food contamination or in any indoor or outdoor environment in which the general public lives. Consequently, depending on the level and route of an individual’s exposure together with her/his susceptibility to a given chemical, life expectancy may be compromised. For instance, the World Health Organization estimated the burden of disease derived from the impacts of selected chemicals in 2019 at 2 million lives lost and 53.5 million disability-adjusted life years. Of those, workers, women, and children are the most susceptible subjects.

In the pursuit of sustainability, politicians, the chemical industry, private and public sectors, and citizens are challenged to collaborate for the paradigm shift civilization needs. Sustainable and circular chemistry are the main tools to enable it. Another significant point to be addressed is from an educational point of view. Both common citizens and chemical professionals (chemists and chemical engineers) need to be taught about sustainability and sustainable/circular chemistry at the earliest in their curricula. Interdisciplinarity among chemistry and other areas of knowledge will be highly relevant within this context. Education also needs to be equally inclusive and integrative among developed, developing, and underdeveloped countries. Additionally, special attention needs to be paid toward reducing inequalities with respect to gender, age, race, and sexual orientation, among other discriminants. All those points are closely related to the concepts from the 17 SDGs from the UN and the Agenda 2030.

The 2030 Agenda for Sustainable Development highlights the reasoning that development must be compatible with the three dimensions of sustainability: economic, social, and environmental (Figure 6). All the 17 SDGs are integrated with each other and are indivisible. In a way, they should be implemented as a whole to guarantee the true sustainable development of society. And, according to the very basic principle of the UN 17 SDGs, the term “society” means “everyone,” so truly sustainable development can only be achieved by considering humanity as a whole, people from all regions of the world, whether developed, developing or underdeveloped, either rich or poor.

Chemical and waste management is essential to the 17 SDGs transversally, offering direction for sustainable chemistry and acting as a universal concept. Targets 12.4 “(by 2020, achieve the environmentally sound management of chemicals and all wastes throughout their life cycle in accordance to international frameworks, significantly reducing their release to air, water and soil in order to minimize adverse impacts on human health and the environment)” and 3.9 “(by 2030, substantially reduce the number of deaths and illnesses from hazardous chemicals and air, water, and soil pollution and contamination)” of the SDGs are directly relevant to a variety of chemical and waste management challenges. It is also important that SDG 9, which promotes the development of resilient infrastructure, inclusive and sustainable industry, and innovation to provide jobs and income, is also important.
Other SDGs, such as SDG Target 6.3 on increasing water quality, necessitate safer chemicals. Finally, some SDGs and targets, such as the ones regarding access to food, clean energy, and secure housing, are directly relevant to chemical-intensive industries. All SDGs and targets have one thing in common: they cannot be met without good chemical and waste management and long-term chemical innovation. As a result, the SDGs serve as a useful guide and pave the way for the advancement of a sustainable chemical agenda as well as circular chemistry. 94,95

4. Circular Chemistry

Some aspects of Green Chemistry, such as atom economy and the environmental factor (e-factor) in chemical synthesis processes, are related to circular chemistry. 34-37 Given that Green Chemistry has been practiced since the 1990s, simplified estimates suggest that industry-wide adoption of some of its innovative principles could reduce global energy intensity (energy used per product per product unit) for the 18 most energy-intensive chemicals by up to 20-40% by 2050 compared to 2010. By 2050, it will mean a reduction in energy of up to 13 exajoules (EJ) per year and a reduction in greenhouse gas emissions of up to 1000 Mt CO₂ equivalent per year. 30 However, those are not good enough. They do not solve the critical economic, social, and environmental issues we are facing today.

Even though Green Chemistry has made major contributions to the improvement of chemical processes in industry and academia in the last 25 years, it is still reliant on the linear economy model and mostly dependent on the single use of nonrenewable resources, which are finite. Furthermore, even by incorporating Green Chemistry principles into many chemical products and processes, they are not at all sustainable.

The Haber-Bosch process, for example, is still used in industrial ammonia production. The disadvantages of this method include significant greenhouse gas (GHG) emissions (more than 2.16 kg CO₂-eq kg⁻¹ NH₃) and high energy consumption (greater than 30 GJ ton⁻¹ NH₃), which are mostly due to the tight operating conditions at high temperature and pressure. 96 According to Ghavam et al., more sustainable alternatives for ammonia production are done through water electrolysis. But it would be necessary to use renewable energy resources (wind, solar, and green hydrogen, among other renewables) for performing electrolysis to be more sustainable. However, it would still be dependent on the availability of (fresh)water, which brings issues related to the water-energy nexus. This high demand for water in a world facing water scarcity would also be prohibitive for several countries around the globe. Furthermore, due to its high volatility, a significant amount of ammonia may be lost by fugitive evaporation, ultimately contributing to altering atmospheric reactivity. Another interesting point regarding the sustainable production of

![Figure 6. The three dimensions of sustainability: economy, society, and biosphere (figure from Stockholm Resilience Centre with CC-BY attribution).](image-url)
ammonia is that it is closely interrelated to green hydrogen production since both are obtained from water electrolysis (and hydrogen can also be obtained from ammonia, in the way \( \text{NH}_3 \) functions as a green hydrogen reservoir). Indeed, some of the authors of the present study are also the authors of another study regarding green hydrogen as a low-carbon energy source. We kindly suggest that the readers interested in the topic refer to that study.

In other words, with the discussion of the possibilities regarding ammonia production, it becomes evident that Green Chemistry, even though it was useful in recent years, is outdated and does not fit well with the needs of a worldwide circular economy model. On the other hand, the models of circular chemistry and circular economy are conceptually inspired by the biogeochemical cycles that regulate the nature and distribution of chemical elements in various environmental compartments. The ideal vision of circular chemistry is for chemists and chemical engineering professionals to promote circularity through interconnected closed-loop processes. In this way, a given “waste” or an “end-product” could be reutilized in the same process or become a resource or feedstock of any other interconnected circular processes, as happens within the natural biological-geological-chemical cycles. To that end, the field of chemistry and related professionals are about to seize a unique opportunity to disruptively rethink and reinvent chemistry through new technologies and innovations with compatibility for circularity and sustainability. Although some good practices from Green Chemistry have some overlap with circular chemistry, their conceptions are different. Since its beginning, Green Chemistry has provided a framework for teaching and performing more sustainable chemistry in industries and academia. This prompted us to consider the development of greener and more sustainable practices, despite the fact that we lacked the concept of considering the entire production chain within circular processes. This reasoning for considering the circularity of chemicals in industry and academia came later, with the introduction of circular chemistry. Indeed, circular chemistry provides an interconnected and holistic view of how the field of chemistry and other chemical sciences can collaborate for the development of a truly circular economy by the end of the first half of the 21st century.

In this way, if, on one hand, within the Green Chemistry scope it is considered the 3Rs rule, on the other hand, circular chemistry has expanded it to the 11Rs rule, stated as reject, reduce, reuse, redistribute, repair, refurbish, repurpose, remanufacture, recycle, recover, and return. Accordingly, similarly to the 12 principles of Green Chemistry, Keijer et al. have proposed the 12 principles of the circular chemistry (Figure 7). This approach is done to facilitate the transition to a circular economy. In this way, it works as a framework similar to the principles of Green Chemistry.
Chemistry. Nonetheless, circular chemistry is an approach to establishing chemical processes to become truly circular and sustainable.\textsuperscript{18,104,105}

According to Figure 7, the 12 principles of circular chemistry\textsuperscript{18,99} can be understood as follows:

(i) Collect and use waste. Reusing waste as a resource is a necessary prerequisite for enabling circularity. Waste is a valuable resource which should be transformed into marketable products in order to promote the (re)circulation of elements, molecules, and materials.

(ii) Maximize atom circulation. Truly circular chemical process platforms should maximize every atom in existing molecules. This requires optimal product design to favor efficient separation and purification steps while enhancing atoms’ reusing possibilities, considering an environmentally friendly route.

(iii) Optimize resource efficiency. Resource conservation should be targeted, promoting reuse, and preserving finite feedstocks.

(iv) Strive for energy persistence. Energy efficiency should be maximized.

(v) Enhance process efficiency. Innovations should continuously improve in- and post-process reuse and recycling, preferable on-site.

(vi) No out-of-plant toxicity. Chemical processes should not release any toxic compounds into the environment.

(vii) Target optimal design. Design should be based on the highest end-of-life options, accounting for separation, purification, and degradation.

(viii) Assess sustainability. Environmental assessment (typified by the LCA, life cycle assessment) should become prevalent to identify inefficiencies in chemical processes.

(ix) Apply ladder of circularity. The end-of-life options for a product should strive for the highest possibilities on the ladder of circularity.

(x) Sell service rather than product. Producers should employ service-based business models such as chemical leasing, promoting efficiency over production rate.

(xi) Reject lock-in. The business and regulatory environment should be flexible to allow the implementation of innovations.

(xii) Unify industry and provide coherent policy framework. The industry and policy should be unified to create an optimal environment to enable circularity in chemical processes.

The 12 Principles of circular chemistry provide a new set of guidelines for the chemical industry and academia to develop a closed-loop, waste-free chemical industry and promote chemical safety. This change of paradigm offers the opportunity to develop novel chemical products and industrial processes that use waste as a resource (waste-to-chemical)\textsuperscript{106,107} and secure a sustainable future by addressing the 17 UN SDGs and Net Zero 2050. One interesting example of a waste-to-chemical process is presented by Antonetti et al.\textsuperscript{107} regarding urea production (waste-to-urea) from the organic fraction of municipal solid waste (MSW). MSW represents an abundant, variable, inexpensive biobased feedstock for producing valuable chemicals, which is likely to improve its economics over its current use. This process is also related to waste-to-energy technologies, since from MSW it is also possible to produce syngas and methane.\textsuperscript{106}

According to Antonetti et al.,\textsuperscript{107} there are several companies already exploring the opportunities from waste-to-chemical conversion. An example is the gasification of waste to synthetic gas, which is also used to produce ammonia and urea.

The use of biorenewable resources such as MSW,\textsuperscript{107} an untapped source of carbon, hydrogen, nitrogen, and sulfur-to name a few elements—could address rising demand for important chemical commodities while also mitigating climate change (because many chemicals would be produced by a non-fossil fuel route) and improve energy security. Depending on regions and lifestyles, the carbon content of solid MSW fractions ranges from 38 to 51\% (average of 47 wt.\% on a dry basis).\textsuperscript{107} The overall organic fraction of MSW ranges from 30 to 50\% by weight. In 2016, MSW output in the Organization for Economic Cooperation and Development (OECD) countries totaled 673 and 278 Mt (total and Europe, respectively).\textsuperscript{106} The MSW amount is predicted to double in the coming years as a result of rising GDP and population, with the global generation rate expected to reach 2.2 billion tons per year by 2025. However, the competition of natural gas production from MSW with the cheaper fossil-related natural gas and oil production, considering the subsidies this type of technology possesses, has become unfeasible.\textsuperscript{106,107} As an alternative to this scenario, the government should seriously consider discontinuing subsidies to the fossil energy sector and directing chemical developers toward cheaper biobased feedstocks whenever possible. By following non-fossil energy production, it fosters a relevant path through circular chemistry decarbonization processes and meets Net Zero by 2050.\textsuperscript{102}

In addition to sustainable chemistry, circular chemistry is intrinsically related to the concepts of chemistry 4.0 and industry 4.0. The following section (section 4.1) will provide more details on the concept of chemistry 4.0. Indeed, new industry 4.0 technologies such as internet of things (IoT), artificial intelligence (AI), machine learning, cyber-physical systems (CPSs), augmented reality and virtual reality (AR/VR) for simulating new processes and
chemical quantum processes, among others, are likely to help the chemical industry achieve leveraged manufacture and improvements of existing processes approaching circularity, as well as by designing new products.\textsuperscript{37,108,109}

4.1. Chemistry 4.0 incorporates digitization, sustainability, and circular economy in industrial chemical processes

The chemical industry is continuously progressing scientifically and technologically with sustainable business model innovations. The term Chemistry 4.0 is related to the concept of Industry 4.0. In the 19\textsuperscript{th} century, the chemical industry began its first period, called Chemistry 1.0, based on coal chemistry and petrochemicals using oil as a raw material. Chemistry 2.0 was marked by scale production and the emergence of new classes of materials such as polymers. Globalization and the production of fine chemicals opened the doors to a new area of industrial chemistry in the early 1980s. That is Chemistry 3.0.\textsuperscript{110}

With recent technological advances, there has been an improvement in hardware and software tools, optimizing chemical processes in industries known as Chemistry 4.0. This digital revolution in the chemical industry has the purpose of sustainable recycling and the circular economy. The plan is to use waste as a renewable source or raw material for new production cycles.\textsuperscript{111} Figure 8 summarizes the evolution of chemistry and the highlights for each cycle.

Falter \textit{et al.}\textsuperscript{112} highlighted that the transition from Chemistry 3.0 to Chemistry 4.0 was marked by radical changes due to automation, specialization, globalization, and the use of renewable materials, biotechnology-aided production, medicaments, new customized products, integrated environmental protection, safety, and health. Figure 9 depicts in greater detail the major changes that occurred during the transition from Chemistry 3.0 to Chemistry 4.0.

The advancement of Chemistry 4.0 will provide innovative solutions to old problems and provide business opportunities for sustainable growth.\textsuperscript{20,113,114} The internet of things (IoT)\textsuperscript{113} is an example of analytical devices that can be described as statements that enable us to conclude that they contribute to a new generation of sustainable analytical methods. Furthermore, studies indicate that by 2040, the global production volume of the chemical industry will almost double.\textsuperscript{20}

Process intensification (PI) strategies are among the necessary actions for transformation in a 4.0 industry.\textsuperscript{37}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure8.png}
\caption{Transition from Chemistry 1.0 to Chemistry 4.0 and its highlights.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure9.png}
\caption{Development from Chemistry 3.0 to Chemistry 4.0 (adapted from Falter \textit{et al.}).\textsuperscript{112}}
\end{figure}
The PI strategy contributes to process sustainability by designing or implementing a novel process or equipment to overcome process limitations in terms of resource/energy and/or waste reduction and/or operational/capital cost. Thus, PI is a potential strategy that supports the circularity of a chemical-based process (new or existing) by reducing the resource utility, cost, and environmental burdens.

In this context, chemistry 4.0 can benefit from systematic adoption of digitalization and digital tools to optimize the management of entire chemical life cycles, from chemical supply chains and chemical manufacturing to use and end-of-life. Chemical processes can benefit from computer-aided methods and tools to develop new processes and services that can meet the needs of society. High-performance computers can play a key role in advancing toward chemistry 4.0. Thus, new modes of computation, such as quantum computing, are receiving more and more attention. Although quantum computing has been in development for some time, the development of the technology to the point of making commercial use of such features is quite recent and still quite limited. There is a rapid development of quantum computing capabilities. In Brazil, for example, there are already quantum simulators for different applications. This opens up potential application areas for academia and industry. So, the advance from classical computing to quantum computing brings with it the solution of relevant problems that were previously unsolvable.

5. Sustainable Chemistry and Circular Economy Concepts Applied in the Industrial Sector: The CCU Example

Carbon dioxide capture and utilization (CCU) is an excellent example of sustainable chemistry and the circular economy. Carbon dioxide (CO₂) is the ultimate product of the combustion of organic matter. It is also produced in fermentation processes and in the decomposition of some mineral ores. CO₂ is presently associated with climate change because it contributes to global warming through the greenhouse effect.

The CCU process encompasses the capture of the gas from a stationary source or even from the atmosphere, purification, and utilization, either directly, such as in the carbonation of beverages, or as feedstock in industrial processes. CO₂ capture may involve four different approaches: (i) absorption; (ii) adsorption; (iii) cryogenic; (iv) membranes.

Once considered a waste and useless product, CO₂ is turning into a valuable raw material for the production of different chemicals and fuels. Technologies for direct air capture (DAC) of CO₂ and its subsequent conversion to fuels, using hydrogen from renewable feedstock and energy sources, are gaining attention all over the world. The forecast indicates that around 30 Mt of CO₂ could be captured from the air and transformed into useful products at pilot and demonstration plants by the end of this decade. This is illustrated by initiatives like CORAL (CO₂ Raw Material from Air), which produces dimethyl ether from hydrogenation of CO₂ captured from the air, and the ProQR, which is a Brazilian-German partnership to produce synthetic aviation fuel.

The Figure 10 below shows some possible applications for the captured CO₂. An example of direct use is in the carbonation of beverages. Fabrication of urea and aspirin (acetyl salicylic acid) are examples of long-term utilization of CO₂ as a feedstock in industrial processes. More recent examples of the utilization of CO₂ as a raw material in the chemical industry are the production of methanol, dimethyl ether (DME), and organic carbonates. While methanol has many uses in the fuel and chemical sector, DME is a substitute for diesel in ignition compression engines, whereas organic carbonates are used to produce polymers and as electrolytes for lithium batteries.

Today, most of the urea produced in the world comes from natural gas, which provides H₂ and CO₂ as raw materials. The so-called blue urea may be fabricated with H₂ produced from water electrolysis using renewable energy, as well as with CO₂ captured from the burning of fossil fuels, providing a good example of how sustainable technologies could be applied to existing products.

Methanol is another chemical that is usually produced from natural gas reforming. Nevertheless, the route using CO₂ is gaining increased attention. An industrial plant in Iceland, from Carbon Recycling International, produces methanol from hydrogen produced by geothermal-driven electrolysis and CO₂ captured from industrial emissions.

Dimethyl ether (DME) can be produced either from methanol or directly from CO₂. Today, most of the DME produced in the world comes from methanol dehydration, which in turn is produced from syngas. However, with the rapid development of the process of methanol synthesis from CO₂, renewable DME is emerging as a potential fuel to replace diesel.

Organic carbonates are important products with uses as electrolytes in lithium batteries, production of polycarbonates, special solvents, and sustainable alkylation agents, among others. An industrial example of the use of CO₂ as raw material in the production of ethylene carbonate (EC) and dimethyl carbonate (DMC) is showed.
in the Scheme 1.\textsuperscript{128} The company uses DMC to make polycarbonates, and this technology has replaced the highly toxic phosgene, the main feedstock used so far. Around 1.7 t of CO$_2$ is fixed and avoided being emitted into the atmosphere for each 10 t of polycarbonate produced, which is a clear and commercial example of a sustainable process.

![Scheme 1. Schematic reactions of the process of ethylene carbonate and dimethyl carbonate production with CO$_2$ as feedstock.](image)

Nevertheless, although CCU could be a promising approach for CO$_2$ reuse and for mitigating its impact on the Earth’s climate, one of the main challenges to implementing projects of direct CO$_2$ capture and conversion is the production of hydrogen, which must be produced from renewable feedstock and energy sources. In this context, water electrolysis or photocatalytic splitting appears to be the most promising when sustainability is concerned.\textsuperscript{129}

6. Challenges and Perspectives

As a result of demographic expansion and the growing demand for goods and services, planet Earth is running out of resources to produce chemicals and materials. Raw materials are only available at high economic costs and with increasing environmental damage. As an essential contribution to a sustainable future, chemistry must be rethought to operate in the circular economy model.\textsuperscript{7}

Although the circular economy paradigm emerged in the 1980s, it was only in the last 20 years that it has gained traction as a more rational and logical way to prevent environmental degradation and, thus, ensure a sustainable world for future generations. However, paradoxically, this model that proposes a more sustainable way of taking advantage of natural resources, manufacturing products, and consumption is finding barriers to its adoption, proving to be difficult, especially to achieve a more comprehensive implementation.

Thus, it is not an easy task to eliminate the traditional linear economic model based on “extract or acquire, use, and discard” and which, in practice, constitutes a “comfort zone” for many people and consumers. However, in the long term, this linear model can be devastating for the environment and, consequently, for life and for human beings.

Several reasons contribute to the difficulty of implementing the circular economy model and circular chemistry, and many...
challenges must be faced in the transition from the current model to a new one based on sustainable progress and the preservation of life and planet Earth.

The main challenges and perspectives for implementing the circular economy model and, especially, circular chemistry, are exemplified below:

6.1. Culture

Consumers are used to the “use and discard” model implemented in recent decades, a system that is encouraged by industry and profit. It is, therefore, necessary to change the way products are disposed of and used, valuing the habits of reducing, reusing, and recycling. This depends on integrated and complementary actions by society, the private sector, and governments through education at all levels, campaigns, and incentives.

6.2. Technology and connectivity

Using advanced technological resources such as artificial intelligence and communication networks is essential to keep up with the advancement of circular economies and circular chemistry. For this, high investments are needed, especially in obtaining relevant data both in the production and consumption phases (life cycle of each product). In addition to the technological resources to carry out the work, it is necessary to qualify people to carry out specialized technical skills.

6.3. Policy and regulation

Many countries already have laws and technical standards that apply essentially to recycling and waste management. However, what is related to ecological development, environmental preservation, product reuse, and consumption reduction, has less stringent policies and does not go beyond informational campaigns and good intentions. It is, therefore, necessary to harmonize the different laws, rules, and regulations existing on the subject, to constitute a legal framework for the circular economy, and to increase its rigor in its application.

6.4. Complexity simplification

Most of today’s chemical products are synthetic, based on non-renewable resources, and are transformed into complex articles such as plastics. Future products and materials must be designed based on sustainability, and it is necessary to restrict the levels of complexity of their constituents to allow recycling.

6.5. Designing products for recycling

Final products should have a composition as simple as possible, minimizing additives and avoiding toxic components that are not easily separated, thus allowing for recovery, recycling, and reuse.

6.6. Chemistry 4.0

Use of renewable materials; biotechnology-aided production to obtain medicines; new customized products; integrated environmental protection; safety; and health.

A good example of the transformation that the chemical industry undergoes is the production of polyethylene (PE), one of the most important inputs in the plastics chain, with a world production volume of approximately 161 million tons in 2015, considering the sum of polyethylene of high (HDPE) and low density (LDPE). In Brazil, there is a company in the chemical and petrochemical sector that is the largest producer of thermoplastic resins in the Americas and a world leader in the production of biopolymers and, since 2010, has had an industrial plant where green polyethylene, the result of the combination of innovation, technology, and sustainability, is produced. Green PE has a low carbon footprint, is produced from a 100% renewable source, from sugarcane, and has the same properties, performance, and versatility of applications as fossil-based polyethylene, and is also recyclable, using the same recycling chain of conventional polyethylene.

Thus, circular chemistry aims to appropriate and use the fundamental scientific knowledge of chemistry in a balanced panorama of the relationship between science and human beings, their surroundings, and their environment. The aim is to develop and innovate chemical methods and processes that maximize benefits while eliminating or, at least, reducing adverse impacts. Therefore, implementing this new model is an opportunity that challenges human imagination and ingenuity in building a better world.

The transition from the linear economy to the circular economy can bring about significant and value-creating changes in many sectors, especially in the chemical industry. The degree and speed of this transformation will depend on the pace of technological development and innovation; the rational use of natural resources; waste reuse and recycling processes; the implementation of public policies and regulatory incentives; new business models; the availability of investments; and consumers’ willingness to change behavior. The gains can be represented by sustainable progress, environmental preservation, and improvements in people’s quality of life.
7. Conclusions

More than ever, it is of a paramount importance to replace the classical model of the linear economy. World leaders, such as politicians, economists and scientists, have advocated a circular model based on making use, reuse, and recycling, to keep products at their greatest usefulness and value throughout their useful life. The “circularity of materials” is emerging as a major focus, as the CE is becoming an essential component in the global economic system to tackle resource depletion and climate change issues. In this context, the circular chemistry may adopt the principles of the circular economy, aiming understand and address the sustainability issues in chemical processes and products, in such a way that the chemical industry can take a competitive advantage provided by the CE, adding value and sustainability in its processes. Although not interdependent, CC and CE are directly related, since the CE is strongly based on renewable materials and waste that, once generated, can also be efficiently recycled or converted into new sustainable products. Finally, the digitization can be a key piece for the sustainable development, in the chemical industry and in the progress of research in basic and applied chemistry, providing the essential support to interconnect new knowledge and technologies with the society’s well-being and wealth.

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Lillian L. N. Guarieiro was responsible for conceptualization, formal analysis, investigation, visualization, writing original draft, writing review and editing; Michelle J. C. Rezende; Williams T. Barbosa; Gisèle O. da Rocha; Pedro A. de Paula Pereira; Daniella R. Fernandes; Wilson A. Lopes; Claudio J. A. Mota were responsible for formal analysis, investigation, visualization, writing original draft and writing review; Jailson B. de Andrade was responsible for conceptualization, formal analysis, investigation, visualization, writing original draft, writing review and supervision.

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