



The circular chemistry conceptual framework: A way forward to sustainability in industry 4.0

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In the framework of sustainability, low-carbon chemistry is presuming importance and consequently, infusion of circular economy (CE) concept will play a vital role to encompass the green/sustainable chemistry principles more comprehensively to the resource-dependent chemical industry. In the present state of environmental challenges, retrofitting the chemical industry with sustainable product stewardship is significantly important. This communication details the much-needed transformation of the chemical industry in the framework of circular chemistry (CC) by adopting the CE concept in the context of emerging Industry 4.0. The drivers that enable the circularity and the methodological approach/tools that help to practice circularity in the chemical industry domain are detailed. The CC needs to inherit the CE principles by employing both life cycle and systems thinking approaches, which helps to understand and address the sustainability issues of the chemical processes/products. The application of the CC concept needs a case-specific protocols developed by a well-defined methodological approach.

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Abbreviations

AIChE, American Institute of Chemical Engineers; CC, circular chemistry; CE, circular economy; CH₄, methane; CI, circularity index; CML, Centrum voor Milieukunde Leiden; CO, Carbon monoxide; CO₂, carbon dioxide; EU, European Union; IoT, internet of things; IPCC-GWP, Intergovernmental Panel on Climate Change – Global Warming Potential; IS, industrial symbiosis; LCA, life-cycle assessment; LCIA, life-cycle impact Assessment; LCT, life cycle thinking; MFA, material flow analysis; PI, Process Intensification; R5, reduce; reuse, repurposing; recycling, and recovery; RAPID, rapid advancement in process

intensification deployment; SDGs, United Nations Sustainable Development Goals; TRACI, Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts; US-DOE, United States Department of Energy.

Introduction

Chemistry is interwoven predominantly with the socioeconomic system since the advent of industrial revolution. The chemical industry is a highly diversified sector based on the heterogeneity in process and product profile but invariably utilizes the fossil based resources such as minerals, natural gas, oil, coal, air, and water as raw materials to produce more than 60,000 different chemical-based products. The diverse applications of these products include in the domain of health, agriculture, transportation, food, energy, environment, consumer products, and so on encompassing product categories of pharmaceuticals, agrochemicals, pesticides, basic and specialty chemicals, fibers, detergents, functional materials, petrochemicals, polymers, and fuels. The customary chemical process follows linear path wherein, a significant amount of raw material is being lost at every step as waste or emissions, which results in huge environmental damage and resources depletion [1]. Chemistry needs to reinvigorate itself as a proponent of sustainable development for providing practical, sustainable, and ethical solutions to the world's persistent challenges by catalyzing radical reforms [2,3]. The chemical sector has the inherent opportunity to take a leading role in combating resource scarcity and environmental crises by way of developing novel/disruptive processes to reuse materials by closed loop approaches [4].

Need to enable circularity in chemical-based industry

Green chemistry allows the optimization of the process by promoting environmentally friendly practices in the chemical based industry within the framework of linear economy [4]. *The Law of conservation of mass and energy* proposed by Lavoisier (1785) and Mayer (1842) says that “Matter and Energy are neither created nor destroyed”. These laws advocate that the available resources on the earth are finite and can not be created or destroyed and therefore, needs to conserve in a sustainable way. Consequently, the ‘circularity of materials’ is surfacing as a prime focus and circular economy (CE) is becoming an essential component in the global economic system to counter the resource depletion and climate change issues. The fundamental emphasis of CE

is to achieve carbon-neutral society by valuing the resources, reducing waste, and addressing the environmental issues in a unified approach [5,6]. Reducing resource consumption, increasing the resource efficiency at all levels of the value chain (suppliers, industry, customers) and extending the life-span of products are the integral components of CE [7]. The practice of CE in the chemical industry can be considered as one of the practical solutions in achieving the objectives of the sustainability [8]. Keijer et al. [4] provided a holistic view on ‘circular chemistry (CC)’ concept based on twelve principles correlating with the green chemistry. Figure 1 depicts the comparative product chain in the chemical industry with reference to conventional and circular practices. Transforming chemical industry to circular practices is quite challenging because of its heterogeneous nature and therefore need to integrate the underlying principle of green chemistry, sustainable chemistry, CE, industrial ecology and Industrial Revolution 4.0 (Figure 2a). CC, in general, is vital at three stages of chemical industry namely, (a) process development, (b) process/product modification, and (c) ‘end-of-life’ scenario. Therefore, new/innovative chemistry is obligatory at these stages of life

cycle to comprehend circularity in the chemical-based industries enabling decarbonization. In this communication, drivers that enable the circularity and the methodological tools that can be used to practice are elaborated in the conceptual framework of CC.

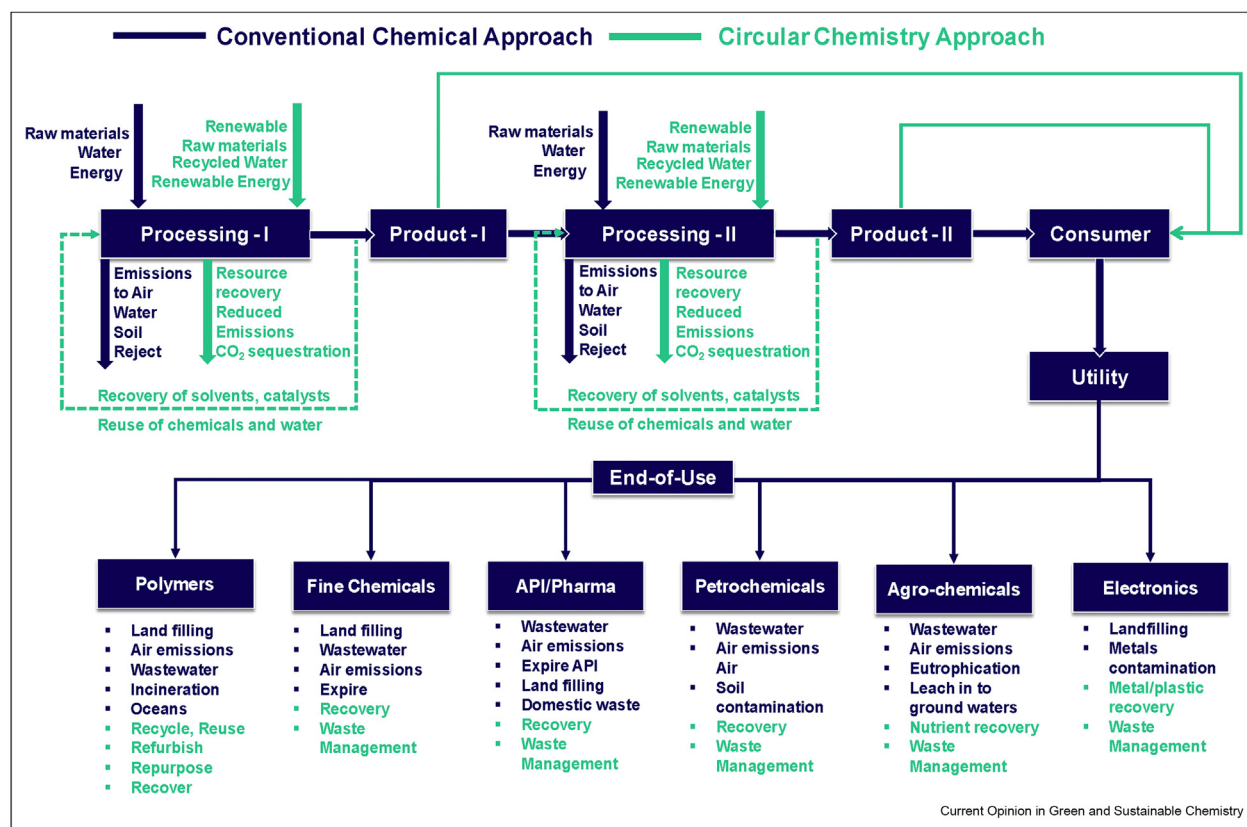
Drivers that enable the circularity in chemical industry

Ten factors which are strategically important and influence a drive towards circularity are discussed herein with reference to the chemical industry (Figure 2b). All the listed elements have complementarity and a well-defined synergy among themselves, and, therefore, cohesive efforts can yield benefits in achieving the overall sustainability.

Closing the loops — molecule circulation

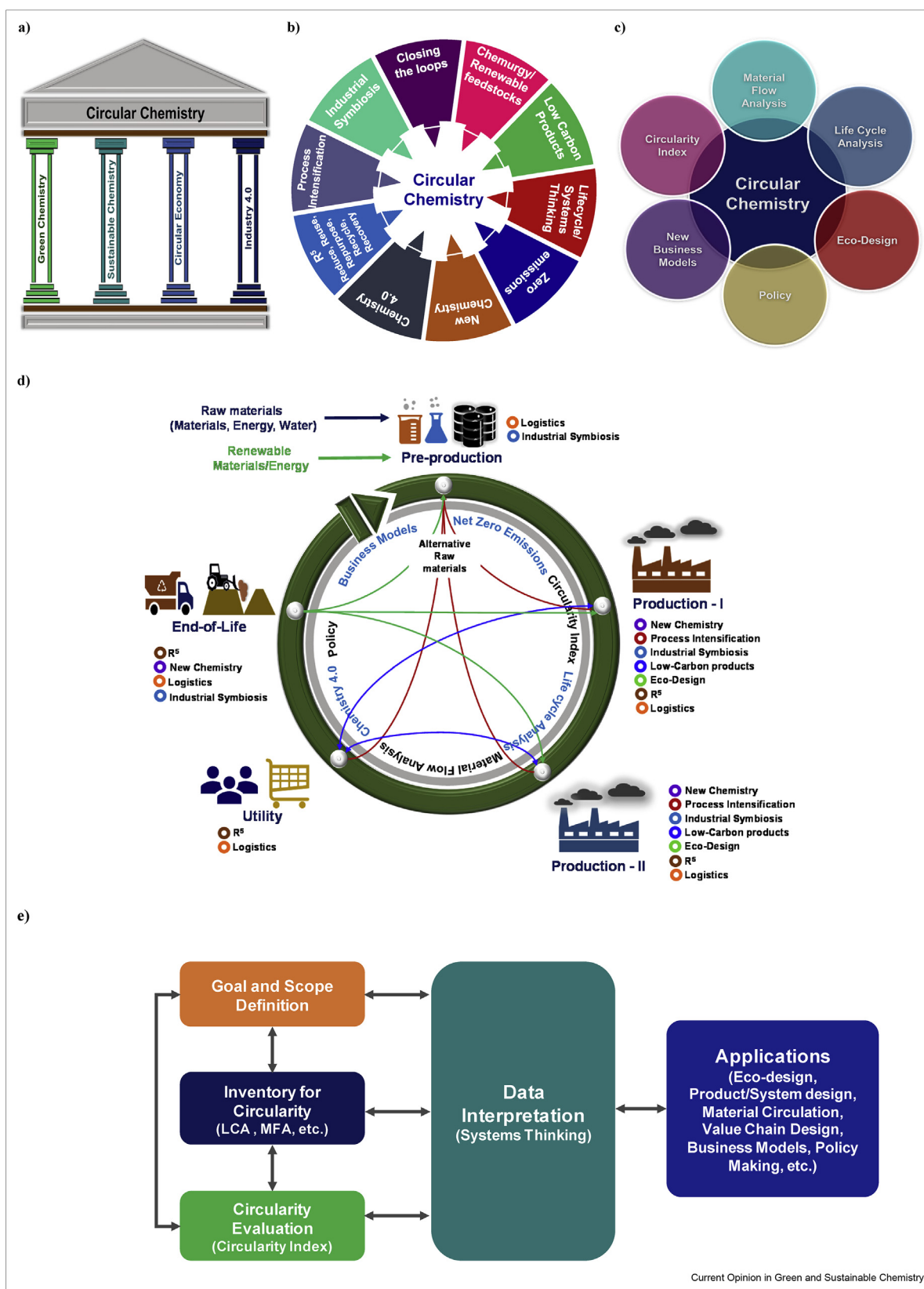
The transition from linear to circular practices is a key driver for the sustainable chemical industry in CE context, which relies on substituting the raw material inputs and redirecting waste into the economic system [9]. The extent of circularity of a process will judge the overall sustainability. Maximizing the materials’ recirculation, increasing the resource recovery efficiency, circular

Figure 1



Transforming chemical process to circular practices with reference to product chain.

Figure 2



Framework of Circular Chemistry. (a) Tangible pillars of circular chemistry; (b) the key drivers that enables circularity in chemical industry; (c) tools that helps to evaluates and design circularity; (d) the conceptual framework enabling circularity; (e) Methodological framework to evaluate circularity.

renovation/innovation, regenerative approach (inducing biological process), and closing the open cycles in a symbiotic way are few key factors that influence the circularity. Closing the open loops, energy efficient practices, and maximal/efficient utilization of residual materials adherently play a key role in this regard [10]. Upon adopting the five archetypal recirculation loops designed by Accenture, near to 60% of the molecules are anticipated to circulate within the EU chemical industry [7]. Circulating the molecules refers to recycling and reuse and is always critical in achieving the required properties or alternatively, finding secondary uses which ultimately needs new chemistry in place [9,10]. MacArthur Foundation has introduced a mass balance principle which helps the industrial sector to become sustainable by circulating the material by looping back within the system to ensure circularity in the chemical industry [50]. However, closing the loops is not only the path to achieve sustainability in a comprehensive way.

Process intensification

Process intensification (PI) strategy will play a decisive role in designing or employing a novel process or equipment to overcome the process limitation with reference to resource/energy and/or waste reduction and/or operational/capital cost, which correlates to the process sustainability [11]. PI facilitates innovating technologies/equipment to improvise manufacturing process with higher product selectivity/purity and reaction rates by optimizing chemical/energy consumption, improving safety, and reducing waste, thereby minimizing the environmental impacts [11,12]. American Institute of Chemical Engineers— rapid advancement in process intensification deployment manufacturing institute supported by United States Department of Energy is intending to develop technologies that enhance productivity and reduce waste generation as well as operational/capital cost related to the chemical manufacturing, oil, gas, and pulp and paper industries [11]. PI can be considered as potential strategy that supports the circularity of a chemical-based process (new/existing) by reducing the resource utility, cost, and environmental burdens [12].

Renewable (chemurgy) — Alternative raw material

Supplementing or replacing the process with renewable or alternative (reprocessed, secondary recycled, and recovered) material in place of virgin fossil-based feedstock (petroleum and natural gas) can facilitate the molecular circulation in a significant way and reduce the dependability on the finite non-renewable resources. In the early 19th century, William J. Hale proposed a concept called ‘chemurgy’ which employs agricultural raw materials as input to link farming with the industry. Chemurgy offered a strategy to crop utilization research in reviving the U.S. agricultural economy during World War II [13], which over the time got decelerated. In the context of green chemistry, introducing the alternative

or renewable materials into the production systems accounts for the low-carbon process/products. Using agricultural biomass/residues is becoming important to counter the finite fossil utility as well as to support the bioeconomy [14]. Biomass itself accounts for cellulose, hemicelluloses, lignin, and renewable sugars (from cellulose/hemicellulose), which functions as platform chemicals in the green synthesis/products [15]. Agri-fats/oils (oleochemicals) can act as potential precursor molecules retrofitting the petroleum-based lubricants.

Low-carbon process/products

One of the primary drivers for sustainability is to achieve the final product with low-carbon footprints in the concept of ‘embodied carbon’, which will account for less carbon emissions throughout the life cycle of product. The final products inherently carry carbon footprints during the whole life cycle starting from raw material procurement, production, transport, and end-of-life [14]. The raw materials should possess low-carbon footprints through sourcing, optimized logistics, and reusability. Using renewable/alternative chemicals (bioethanol, lactic acid, sugars, lipids, and gases such as H₂, CO₂, CH₄, CO, etc.) in the production will account for the low-carbon process or products [51]. Energy is an important entity that significantly adds carbon footprints during the process life cycle. The chemical industry contributes to 10% of the total global energy demand, where the major fraction is derived from fossil-fuels [16]. Energy consumed at each stage (resource extraction, processing, production, logistics, and end-of-life) contributes to the overall emissions [17]. Energy efficient strategies and infusing renewable energy into the process can facilitate for lower embedded carbon. Adopting PI practices can also assist in the sustainability of process to a considerable extent [14]. Extending the product life span, reducing the dependency on virgin material, local sourcing/supply of raw materials, infusing renewable energy, the extent of material recovery and circulation, energy-efficient practices, process efficiency, and CO₂ utilization are some of the essential factors that account for low-carbon process [14,15]. The acceptability, applicability, recyclability, and trading of the alternative/secondary raw material are the major factors for the regulation of circularity in the chemical industry [15].

Five R (R⁵)

Five ‘R’ namely reduce, reuse, repurposing, recycling, and recovery will play a decisive role in assessing/achieving the overall circularity in chemical-based industry. However, because of its high diverse nature, adopting the R⁵ will vary from case to case (Box 1).

Net zero emissions

The global chemical industry is switching towards achieving zero-emission goals, which is indispensable in

Box. 1. The application of R⁵ to circularity in chemical-based industry

Reduce: Chemical industry consumes a large number of reagents and solvents which eventually result in waste. The material utility can be achieved by simplifying the reaction steps, reduction of other derivatives, increasing product lifespan, and minimizing the logistics [1].

Reuse: Conservation of finite resources needs to be fostered by promoting the reuse of the unreacted materials (catalysts/solvents/reactants) in the production for multiple times. New technologies for continuous reuse of materials within the system or industrial park (symbiosis) need to be infused [18].

Repurposing: Repurposing is the modification or revision of a product to function for a new application or in other domains that helps to reduce the end-of-pipe waste, redeems cost/materials, increase renewability, and durability [4]. The repurposing of the products through chemical/thermal/biochemical methods reduces the requirement of primary feedstock, optimizes the resource yields and increases multifunctionality of products [9]. Repurposing of metal/alloys, plastics, electronics, mineral oils, solvents, and vitamin supplements is in general practiced [19].

Recycling: Recycling aims at sustainability thereby promoting circularity. Recycling (mechanical/chemicals) prevents waste and reduces virgin raw materials consumption [8]. The recycling of material relies on the retrieval of its native properties, wherein new chemistry is indeed essential. Recycling of metals, materials, solvents, and chemicals accounts for resource-efficient practices. The recycling process not only supports the environment but also is justifiable with societal and economic factors.

Recovery: Recovery is intended to recoup the energy/material which exists after recycling process, through thermal, catalytic, or biological processes. Solvent recovery by distillation techniques, pervaporation, and nanofiltration are the common practices used in chemical industry. Biological recovery practices namely anaerobic digestion, acidogenic process, algal cultivation, and so on helps to recover the resources from waste/wastewater [20].

achieving the circularity. The chemical sector evolved as one of the sizeable contributors to the global emissions, wherein plastics production solely is projected to occupy a share of 15% of the worldwide annual carbon emissions by 2050, where nearly 2.7 tons CO₂ may be released from burning of one ton plastic waste [21]. Therefore, reducing the process emissions is one of the prime criteria that accounts for the success of the circular practices. ‘End-of-life’ considerations need to be balanced against product performance by giving less priority to ‘end-of-pipe’ treatment or low-value waste management [5]. New/innovative chemistry is required to play an important role at this stage to valorize the resource recovered, similar to the production stage. Utilizing gaseous emissions towards value addition is a new domain of interest apart from liquid and solid waste valorization in the format of biorefineries for products that can supplement to the production chain [15,20].

New chemistry — innovative technology

In the context of CC, new chemistry is critical at three life-cycle stages (a) process development, (b) process/product modification, and (c) ‘end-of-life’ scenario. Innovations in chemistry are much needed during designing of new products with high selectivity/recyclability and in developing a new process that can recycle byproducts into molecules with specific application [5]. Chemical recycling of materials (polymers/plastics) demand new chemistry to improve reuse and recycling contrary to the mechanical recycling [22]. Reducing the cost of reusing materials (reverse-cycle) and recovering resource from waste based on a life-cycle approach is critical [7]. In general, the components in the waste streams are difficult to separate and needs new chemistry/recycled means. Advancement in industrial biotechnology leads to use of sustainable materials in the production process. Biotechnological interventions (biologization of chemistry) in chemical-based industries can play a major role in achieving sustainability [22]. Bio-transformations (microorganism/mammalian/enzyme systems) positively impacts the efficacy and safety of the product [23]. Biology-driven approaches can complement medicinal chemistry in drug optimization and also synthetic biology strategy will provide an alternative route for producing chemicals and its analogs [24]. Semisynthesis (partial chemical synthesis) can be adopted when the precursor molecule is structurally complex, or costly or inefficient is one major application. Semisynthetic chemicals produced either by modification of a natural material or by combining chemicals with natural components as a hybrid is a potential alternative [24,25]. Disruptive technologies offer opportunities for new areas in the chemical sector that can significantly alter the way consumers, industries, or businesses operates [22].

Industrial symbiosis

Industrial symbiosis (IS), a sub-discipline of industrial ecology, is an integrated approach that promotes the reuse of wastes/by-products generated in the process on a local level, through sharing/leasing by reducing logistics and therefore, support CE [9,14,26]. IS replicates the functions of ecosystem by networking all the colocated companies to offer circulation of materials/energy within the system itself with minimal losses [27]. It encourages in synergizing the output from one process as input for other process(s) in the given system, fulfills the goal of CE [8]. In this context, LCA facilitates to assess the symbiotic network among the system by quantifiable analysis of spin-off/by-product to share in a rationale way [28]. The IS offers value to the waste material and tangentially favors both environmental and economic reserves and, therefore, facilitates the development of circular business models [14]. The Kalundborg Industrial Symbiosis Complex is one of the finest

Box 2. Methodological tools that can be employed to evaluate circularity

Material flow analysis (MFA): MFA facilitates precise quantitative flows and stocks via mass balance check and sensitivity/uncertainty analysis which helps to identify the process hotspots and forms basis for the decision-making [35]. The MFA with accurate data assists in guiding the circularity approach to be practiced in the defined system by assessing the material flux in a specific time interval. The analysis will help to identify the snags in the processes and provides signpost pathways to address the material losses in the system. MFA as a methodological tool enables the industry to comprehensively regulate the flow of materials and energy by adopting resource-saving practices and loop-closing strategies, thereby tend to reduce waste generation [36]. MFA influence the waste management practices, environmental impact evaluation, and policy-making [3,37]. It directly helps to manage resources, wastes, and environmental issues resulting in establishing a sustainable process [38]. It also helps in selection of potential in-use stock products, tracing the drivers of circularity, backfilling of nonhazardous waste in the product chain, optimizing materials and energy flows and conservation of materials in co-located processes [39]. The MFA also provides a viable inventory data for LCA.

Life cycle analysis (LCA): LCA evaluates the sustainability metric of a process/product across the defined life cycle boundary and also identifies the inefficiencies and hotspots [14]. It operates on inventory data as input (raw materials, water, and energy) and outputs (targeted products/by-products and emissions at each step) as per the guidelines of ISO14044:2006. LCA provides environmental impact information of a product throughout the life cycle based on the impact categories and thereby identifies the hotspots. The system boundary selection ('Cradle to Gate', or 'Cradle to Cradle', or 'Gate to Gate') is key in assessing the impact [15]. The impact can be assessed by employing various LCIA methods namely IPCC-GWP, TRACI, Impact 2002+, Ecoindicator99, ReCiPe, CML, etc. [14]. Impact 2002+ method depicts the impacts concerning to 14 mid-point categories and four end-point damage categories (namely, human health, ecosystem quality, climate change, and resources) [40]. IPCC-GWP method evaluates the influence of the product/process on the global warming (in kg CO₂ equivalents). The contribution share of each input on various impact categories can be represented in the form of Sankey diagram. LCA implementation during the process optimization (before scale-up) or production design and implementation stages or during process intensification/modification will provide a comprehensive input on the environmental setting thereby helps to minimize the impact [41]. This also helps to understand the inefficiencies in the current processes and guide towards the process intensification. The LCA report will provide insights that help in considering specific key performance indicators that prop up the circularity scenarios [14]. LCA also finds the prospects in the framework of industrial symbiosis.

Circularity index (CI): The circularity of a system is estimated with various indicators by managing the transition of the materials and energy at different stages of the production chain and strategies oriented toward products (end-of-life extension) [42]. The indicators need to prioritize the environmental, societal, and economic outcomes of the process, where all the relevant data need to be incorporated holistically [43]. CI need to be embedded with key aspects such as resource productivity, recyclability, and reusability of the materials/energy, inputs (virgin/recycled/biobased), lifespan, end-of-life use (recycle/incinerate/landfill), and the recycling/reusability efficiency [44]. Various studies confer that a set of indicators or composite indicators are mandatorily employed to assess the CE instead of an individual indicator to explore the integrity [34]. Together with the circularity prospects, the secondary emissions should be considered, where sometimes these may lead to unexpected and potential issues [44]. Design and development of circularity index specifically for each category of industry helps to quantify the overall circularity achieved by the selected process in a defined boundary.

Eco-design: The eco-design concept integrates the environmental conservation aspects to each stage of the product's value chain. According to ISO 14006:2011 guidelines, the products of eco-design need to be versatile, opportune to reuse and recycle, lower environmental impacts, compact (consumes fewer materials and fuels), efficient, and sustainable. This design approach pays attention to production with fewer materials and energy inputs to conserve resources and reduce emissions. Optimum resource usage, utilizing materials that are reused/recycled with biodegradability and durability, extending the lifespan, and awareness in the users [45] are some indicators that significantly intervene eco-design. LCA can be employed to evaluate the environmental performance which also serves as a tool in validating sustainability before the scale up operations [46]. Embracing the eco-design approach with IoT technologies in the context of Industry 4.0 consistent with CE could be a compelling strategy [47]. The cross-discipline collaboration among science and engineering helps to introduce innovation strategies for sustainable product design in the chemical sector.

New Business models: The linear economy will gradually become more circular when circular value chains become more competitive [7]. The main challenge with CE is to perceive the applicability and growth through new business models [10]. The five business models namely, circular supplies, resource recovery, product life extension, sharing platforms, and product as a service are discussed by Accenture [7,48]. The models foment the alternative material use, resource-efficient production, energy recovery and efficiency, extended product life cycle, switching to chemical leasing models, and service-based sales [10]. To develop a dynamic business strategy and to generate profit, the industry needs to consider the circularity advantage of the product chain/system [48]. Industry 4.0 needs to infuse the circular practices in production and trade that effectively confront the potential SDG targets [49]. The European Green Deal has set an action plan to enhance the resource efficiency by switching to a clean and circular economy to bringdown the pollution and to achieve carbon neutral by 2050. The plan features the CE economy transition as core component and promotes new business models with requisite investments and financing tools [52].

Policy: A defined policy and regulatory framework are pre-requisite to infuse and practice circularity in any of the industrial settings. The policy should provide an economic incentive or green rating/grading to the operators adopting the circular practices with zero emissions. The use of alternative materials in place of fossils needs a defined policy and regulation. Encouraging the industrial symbiosis in the framework of eco-industrial parks needs special focus. A cohesive and systematic road map to achieve circularity in the chemical industry with a long-term guiding plan and policy is essential.

examples of IS and many eco-industrial parks are emerging with IS concept around the globe.

Life-cycle (system) thinking

Systems thinking and life-cycle thinking approaches can aid in reinventing the chemistry, and form a basis for developing sustainable chemical products/processes that contribute to realizing the CE [4]. The approach of systems thinking facilitates the inter-relationships between the biological and physical environments of the planet, beyond solving immediate and separate problems by considering many factors together including sustainability and ethics [29]. Product or process needs to be measured in terms of its contribution to ecological, societal, and economic aspects, based on the conservation of resources, health, safety, and cost efficiency spanning the entire value chain [30].

Chemistry 4.0 — embrace digitalization with circular economy

The chemical industry is being continuously progressing with scientific and technological innovations with time. Specifically, Industry 2.0 evidenced mass production due to possibility of upscaling and modernization with the advent of petrol chemistry. Chemical industry during Industry 3.0 encountered a radical change due to automation, specialization and globalization along with use of renewable materials, biotechnology-aided production, new and customized drugs/products, integrated environmental protection, safety, and health aspects [31,32]. Now, advancing Industry 4.0 with the digital transformation is marching towards conservation of materials/energy incorporating CE as the core enabler for the overall sustainability. It is believed that Industry 4.0 has the potential to transform the chemical industry by streamlining operations with the help of digital analytics, wherein circularity forms an important entity that can be linked to digitalized business models [33].

Tools

Specific indicators and tools are obligatory to assist the practitioners in assessing the circularity in the chemical sector which ultimately helps in both decision and policy making [34]. Diversity of processes, products, applications and end-of-life scenario are the snags for the design of a generalized methodology to assess/practice the circularity in chemical based industry. However, six methodological tools namely, material flow analysis (MFA), life cycle analysis (LCA), circularity index (CI), eco-design, new business models, and policy have a direct role in assessing and designing the circular and sustainable practices are discussed herein (Figure 2c; Box 2).

Way forward

The diversity among chemical industries, product profiles, their specific applications, and the end-of-life

variations make the sector more complex and therefore, arriving at a unified methodological approach for assessing circularity is challenging. The circularity of a system is to be established with components such as extractive operations, logistics, process, generation of waste, resource efficiency, environmental impacts, business models, and policy [10,14]. Life cycle thinking with a systems approach is important to assess the impounding sustainability aspects of a chemical process to calibrate circularity. LCA and/or MFA tools will help to assess the hotspots and addresses the sustainability aspects specific to the process that can looped back within the system or to redesign the system with ecological perspective [14]. Figure 2d and e depicts the conceptual and methodological framework proposed respectively, to enable the practice of circularity in chemical-based industry. Chemistry needs to play a critical role throughout the life cycle especially at the end-of-life operations to circulate the potential material that has prime application in the industry or in a symbiotic mode in the framework of industrial ecology. New business models, policy, and subsidy also majorly influence the implementation of circularity.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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