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Sustainable Chemical Technologies for Clean Energy, Water, and Environment: A Systems Thinking Perspective

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Abstract

The continual provision of basic needs such as energy, fresh water, and a healthy living environment, alongside the protection of natural ecosystems, is a grand societal problem. It is especially crucial to meet these needs, popularly referred to as the sustainability grand challenges, given that the world population is increasing, economic growth is accelerating, natural resources are being depleted rapidly, and the climate is changing rapidly. The global chemical industry is central to grand challenges related to sustainability, as it provides a broad range of chemical solutions for energy supply, water quality, and water pollution prevention. However, it is necessary to evaluate and make decisions about chemical solutions at the systemic level and their trade-offs. Most of the solutions have debilitating drawbacks or are still too immature in science, despite their good potential. Thus, the dynamics, interactions, and feedback among these energy, water, and environmental factors within a more extensive system context become key to preventing the intentional actions that lead to unwanted side effects in other parts of the socio-technical system (Schlögl, 2016). Grand challenges of sustainability may thus be regarded as interconnected. It is risky to address one challenge without considering how it might affect other challenges. Chemical technologies will add pressure at the systemic level but typically create additional problems (Summerton et al., 2019). Hence, it is possible to identify systemic effects of chemical innovations at an early stage by characterising the source-process-end-user materials flows that underpin these challenges. Specific chemical solutions that effectively address sustainability grand challenges and their consequences for a system have emerged as a viable field of study. Numerous innovative technologies are already commercially available and *risk creating unanticipated collateral effects on sustainability. To address such solutions, a systems approach to chemical innovation and technology development is required.*

Keywords: *Sustainable energy, green chemistry, circular economy, electrochemical processes, wastewater treatment, hydrogen economy, life cycle assessment, systems design.*

1. Introduction

The sustainability of the chemical technologies that help address the problems of sustainable development will become the key to the continued availability of the most vital services, such as energy, water, and a livable environment, in the second half of the twenty-first century. Exploration and analysis methodologies grounded in systems thinking can accelerate technology research and development by identifying the most critical steps and potential solutions while accounting for unintended and interdependent effects. Systems thinking is necessary because of technical, regulatory, and fiscal issues that chemical technologies face in finding a place in sustainable energy, sustainable water, and sustainable environment solutions; these issues can only be met and solved at the systems level. In general terms, the following paper aims to provide an overview of the connections between systems thinking and the sustainability of chemical technologies, identify the relevant principles, questions, and arguments, review past directions in the technology's exploration, and outline new research directions.

Renewable energy generators, which are technically and economically viable, are replacing fossil fuels. The other problems of seasonal and daily imbalances, uncontrolled co-production of H2 and dimethyl ether (DME) from syngas, stabilisation of CO2 levels, and the collective responsibility for an energy carrier such as hydrogen (H2) are still not fully resolved. Decision-support systems, consumption-monitoring techniques, and energy carriers are necessary to provide flexibility in demand-side energy management when these systems are distributed, off-grid, and enhanced to achieve energy efficiency (Schlögl, 2016).

The effectiveness of chemical technologies aimed at the sustainable availability of energy, water, and an environment that supports life is studied separately in both academic research and industrial development. The challenges and research questions associated with them, as well as the state of exploration, are outlined, drawing on examples from various technological fields.

2. Basic Principles of Sustainable Chemical Technologies.

Green chemistry is a new trend that has emerged to fight climate change, water scarcity, and pollution. Nevertheless, many of them are impossible due to technological, economic, and social obstacles. Such barriers may be identified and addressed with the assistance of a systems-thinking perspective, thereby creating opportunities for a wide variety of chemical innovations that will spur global sustainability and extend beyond energy, water, and the environment. Systems thinking provides a methodical understanding of the boundaries of technology systems, the relationships between system components, changes in behaviour over time, and sustainability measures. It therefore serves as an important complement to the analytical methods commonly employed in chemical engineering, such as mass and energy balances, or the design of experiments. It is very much in keeping with current trends toward more integrated research and development plans.

The concept of sustainability provides a good starting point for relating sustainability aims to chemical innovation. Sustainability involves the long-term conservation of essential, critical, and non-renewable resources and the reduction of adverse effects on human health and the environment. Collectively, these dimensions determine zealous goals of industrial processes. The Green Chemical movement has sought to establish sustainability principles for chemical production. Even though these principles were initially applied to the synthesis of chemical products, they are now being acknowledged as applicable to broader sustainability issues. Beyond these, more holistic measures have been suggested to generalise green metrics across systems and processes, to offer cradle-to-grave analyses of resource consumption and emissions, and to inform process designs to maximise resource performance and related emissions, all of which are questions of paramount significance in sustainable development. These systemic extensions are also in line with the new vision of Green Chemistry as the accountable handling of obligatory chemical materials to serve the community and the ecosystems, rather than the absence of chemistry (Ibrahim Samli, 2011).

2.1. Sustainability Principles in the Process of Chemicals.

Sustainable chemical processes and unit operations should be designed to harness renewable resources with minimal environmental impacts, including water and energy use, pollutant generation, and the generation of solid, liquid, and gaseous wastes. The current trend in sustainable technology design is the incorporation of green chemistry and engineering principles, natural resource use, and the reduction of resource use and waste treatment into the sustainability of chemical processes and the choice of chemical products (Ibrahim

Samli, 2011). The reduction of toxic vapours and the generation of wastewater are also highlighted, as these indices correlate with other pollution prevention measures and are based on technical and economic factors. Based on the corresponding analysis, another viable option to the existing manufacturing processes is the use of so-called dispersed catalysis, inspired by chemical ecology and the latest catalytic processes.

Both processes and products should be designed to reduce the natural toxicity of feed, auxiliary, solvent, and product materials. The chemical's toxicity is also denoted by the type of use, probable exposure level, concentration, and duration. Therefore, wider toxicity ranges are used to interpolate and simplify assessments based on available hazard scales for chemistries. Generation and treatment focuses of wastewater are also key pollution indicators. As a result, a small-scale methyl chloride synthesis system using paraffin as a feedstock in a portable, small-scale setup, without the need for excessive production of contaminants and their subsequent large-scale purification, is created.

2.2. Chemical Innovation Systems Thinking.

The concept of chemical innovation is based on sustainability principles that ensure the sustainable and efficient use of resources throughout the life cycle (Jen Mendelsohn Matus et al., 2013). In short, greener technologies can be used to provide sustainable water solutions with the help of sophisticated materials to treat drinking water, upcycle wastewater, and transform seawater into fresh water; recover resources from waste streams; and treat water in manufacturing processes. The energy technologies that facilitate the electrification of industrial processes without skyrocketing electricity bills require catalysts that enable the conversion of carbon-based feedstocks into sustainable energy or chemical feedstocks (Schlögl, 2016). The potential of systems thinking to advance the idea of sustainability in chemical engineering is evident in its ability to evaluate nonlinear interactions, integrate quantitative and qualitative arguments, adopt a multi-stakeholder point of view, and address technological evolution over time.

The long-held connotation of systems thinking with mathematics is misleading to its broader meaning as a heuristic concept capable of tackling the complexities of the change machine and the economic system, as well as the contextual forces behind the evolving sustainability demands in chemical engineering. Systems thinking narrows down the constituents that make up a complete chemical process and necessitates looking at by-products as waste. It is a chemical engineering method that includes inputs, outputs, functions, nature, and boundary conditions, which strongly combine energy, water, and environmental interactions with limited resources. In many fields, loyalty to the set process boundaries does not allow attention to shifting sustainability standards, which is why the food-energy-water nexus and the connection between chemical engineering and the energy transition and circular economy challenges make sustainability even more challenging. These principles can contribute to a more holistic view of the background determinants, further supporting sustainability-oriented programs as more people expand the definition of sustainability.

Sustainability acknowledges the interaction between long-term socio-economic development and the preservation, conservation, and renewal of natural systems, to achieve the well-being of ecological systems for both the current and future generations. Three generic sustainability ideas underpin the creation of the overarching sustainability tenets: the planet cannot sustain unchecked consumption; growth cannot continue indefinitely on a finite planet; and the whole population cannot be lifted at the expense of the Earth's systems. The resultant emphasis on the toxicity of chemical operations, as reflected in sustainability principles relevant to the specific case of chemical engineering, is directly related to the essence of chemical engineering itself and directly connected to the ever-tighter laws and regulations imposed on nations, regions, and fabricators.

3. Sustainable Energy Technologies.

Sustainable energy landscapes may be enhanced using a broad spectrum of chemical technologies. Sustainable chemical energy technologies have been developed to provide electricity from renewable sources, generate power in an ecologically friendly way, store energy from regenerative resources, and produce renewable heating and transport fuels. These technologies are evaluated within a systems framework that considers their interdependence with water resources and environmental quality.

The energy technologies that enable the shift to a sustainable global economy are chemical in nature. It is expected that the energy sector will be structurally decarbonised to meet climate goals and prevent irreversible environmental harm. Natural systems should be sustained by supplying sufficient energy in diverse forms and vectors to meet demand. The implementation of renewable energy resources and energy storage systems will meet society's energy needs. However, decarbonising the economy without a clear initiative to replace heat sources in industrial processes and land

and air transportation with renewable ones would significantly undermine global warming goals. Another important solution is to improve energy efficiency, and, as a result, the roles of electrification, the utilisation of low-grade heat, and the implementation of carbon capture and storage (CCS) technologies will become central to reducing emissions.

Hydrogen is the safest form of energy to transport over long distances, and can be produced using renewable sources with zero emissions. Its methods of utilisation range from those capable of accepting relatively low-purity streams to extremely pure streams, to large-scale applications that require gas with a satisfactory but not very high level of purity. Moreover, hydrogen can be part of decarbonization efforts, as it can provide renewable fuels, including methane and hydrogen-rich hydrocarbon liquids, for high-temperature industrial applications and terrestrial transport. However, hydrogen has a low volumetric energy density and requires a lot of energy to liquefy, whereas ammonia is difficult to handle because it is extremely toxic and corrosive. It is necessary to note that natural ecosystems will not provide hydrogen for the circular economy; human activity will have to produce it.

3.1. Photoelectrochemical Systems and Electrocatalysis.

Reduction technologies, including electrocatalytic and photoelectrochemical, are essential for addressing the energy crisis and environmental issues. Electrocatalytic systems convert renewable electricity, given its intermittency (e.g., wind- or solar-generated electricity), directly into chemical energy. Photoelectrochemical (PEC) devices do not require electrical power at all, but can internally convert renewable energy sources, such as solar, wind or biomass, into chemicals. The most appropriate solution for energy storage is solar-to-chemical conversion, as it utilises the planet's abundant, renewable solar energy and can be integrated with existing infrastructure.

The kinetic parameters, including material stability, product selectivity, and catalyst efficiency, are required for the conversion of CO2, H2O, nitrogen-containing compounds, and organic pollutants into value-added chemicals and renewable energy fuels. When chemical production involves complex separation processes and treating highly dilute aqueous waste streams, electrocatalytic and PEC systems capable of coupling to renewable energy are also required. The essential qualities affecting the performance of electrocatalytic and photoelectrochemical systems, such as catalysts, materials, efficiency, stability, and adaptability to specific renewable energy sources, must be assessed to enable systematic analysis (Kaeffer & Leitner, 2022; Zhang & Wu, 2024).

3.2. Renewable fuel conversion catalytically.

A systematic and thermodynamically favourable chemical conversion of biomass-based feedstock into hydrogen and carbon dioxide constitutes the white space for catalyst development. Natural oil converted into industrial products through catalytic conversion by industries is well documented to have been made using dinosaur-age biomass. Hence, the manual tracking and optimisation of the renewable conversion technology, in which the sustainability road map is the dotted line on the way to the seemingly expected final product, allows a more articulate, distinct, and comprehensive evolutionary account of each catalysis. The white-space illustration is to some extent obscured by the intermingling of natural oil and biomass, as well as the unavoidable, large-scale controversy surrounding methanol-to-olefins (MTO) that must be illustrated. However, the preparation of the complete and pure renewable catalogue adjacent to the wooden building still allows an uninterested, goal-oriented upgrade of the solar-driven, steady-state whole-conversion trace across the chemical, materials, catalysis, reactor, and system disciplines, and the discipline-related considerations constitute another stratum in the catalytic science of ochre.

Biomass feedstocks are also examined for catalytic conversion into different quantities of hydrogen (H2), carbon monoxide (CO), carbon dioxide (CO2), chemicals, and/or fuels (G. Yadav et al., 2020). However, the alternative application of biomass or biowaste as a safe-drop or a dummy feedstock across the entire value chain, to decarbonise the economy, was threatened by chemical, infrastructure, and environmental incompatibilities. Full-cycle consideration confirms the direct conversion of biomass into intermediates, with methanol and middle olefins characterised as the best gateway to current global demand. Biomass-to-methanol (BTM) and methanol-to-olefins (MTO) two-way coupling to design large-scale conversion plans is therefore possible.

3.3. Energy Storing Materials and Processes.

Given the decarbonization of the energy system and the growing use of renewable energy sources, energy storage has become a priority in technological terms worldwide (Ausfelder et al., 2018). The scientific interest of various players lies in the safe, sustainable, and democratically distributed storage, release, and conditioning of energy in its various forms. The fact that the entire system, including energy supply, storage, and release, and user demand, is important to consider, especially in the interactions and synergies among the various components.

Storing energy opens possibilities to make current energy-consuming devices smarter and, through open-source, to share technological knowledge across interinstitutional and geographical borders. Of primary importance is the operation of the whole system, including processing activities such as storage with batteries or supercapacitors. Therefore, new materials to enable such energy storage and release, e.g. technologies based on battery-, supercapacitor-, or fuel-cell-like materials, are required (de Jesús Illera Perozo, 2019). Durability and environmental impact are two important parameters under consideration in broad-based contexts, such as laboratory cell experiments, small-scale systems in fleet vehicles, and infrastructure in smart cities. The substances should be sustainable, inexpensive, low-impact on the environment and recyclable after use (Kaylie Stauffer, 2016).

Table 1: Sustainable energy technologies in a systems perspective

Technology	**Input/feedstock**	**Main products/service**	**Key sustainability advantages**	**Major system-level limitations**
Electrocatalytic CO_2 / N_2 / H_2O conversion	CO_2, N_2, H_2O, renewable electricity	Green fuels, chemicals (e.g.,-fuels, ammonia, alcohols, etc.)	Direct coupling to intermittent renewables, low-temperature operation	Catalyst stability, selectivity, scale-up and infrastructure gaps
Photoelectrochemical (PEC) systems	Sunlight, CO_2 / H_2O, semiconductor materials	Solar-to-fuel (H_2, hydrocarbons), value-	Direct solar-to-chemical conversion, potentially high efficiency	Materials degradation, low practical efficiency,

Technology	**Input/feedstock**	**Main products/service**	**Key sustainability advantages**	**Major system-level limitations**
		added chemicals		and the cost of devices
Biomass-to-methanol (BTM) and intermediates	Biomass/bio waste feedstocks	Methanol, middle olefins, platform chemicals	Utilises renewable carbon, integrates with existing petro-infrastructure	Feedstock variability, logistics, land-use and food–fuel concerns
Energy storage (batteries, supercapacitors)	Electricity, active materials, electrolytes	Stored electrical energy, grid balancing, e-mobility	Enables high renewable penetration, demand-side flexibility	Critical materials, recycling challenges, lifecycle impacts
Hydrogen as an energy carrier	Water, renewable electricity or low-carbon fuel	H_2 gas/liquid, hydrogen-rich fuels	Long-distance energy transport, sector coupling (industry, transport)	Low volumetric density, liquefaction energy, safety and handling

4. Sustainable Water Technologies

The global issues that have had a devastating impact on human health and well-being include water scarcity, pollution, distribution deficits, drought and flooding, and climate change in cities (Fairburn et al., 2017). A more thorough approach to water will help create a more detailed understanding of the water-energy-food nexus and develop a more sustainable solution. Chemical technologies are very important throughout the water cycle, and multiple methodologies have been proposed to clean water, extract resources from wastewater, generate fresh water from marine sources, and treat micropollutants widely distributed in the environment.

Water quality and water resources are regarded, which also encompasses water purification and treatment catalysis, desalination, and resource recovery, as well as wastewater valorisation, including upcycling routes, potential value streams, and inclusion in circular economy flows (Alan Hatton et al., 2017). This is because projected population growth and water demand have prompted the use of desalination as an alternative water supply and a valuable source of chemical feedstock. With or without its inseparable high-energy intensity and salt by-products, a whole world of opportunities remains in the water-energy-food nexus and beyond, regarding catalysts of choice, coupling with renewable energy, and valorising by-products.

4.1. Water Purification and Treatment Catalysis.

The use of chemical processes offers a wide range of options for reducing water contamination, managing water resources, and promoting hygiene by treating a range of contaminants across different media (Alan Hatton et al., 2017). Researchers are interested in microbial fuel cell technology, biochemistry, and electrocatalysis as areas that can effectively eliminate contaminants in water (Zhang et al., 2024). Direct catalytic treatment of wastewater is also not a commonly used method for removing contaminants. Efficient treatment can be enhanced by installing well-designed photocatalytic or electrocatalytic systems that are integrated after physical filtration. There are numerous chemical water treatment technologies, and chemical catalysis is necessary in most of these. Despite the challenges of producing catalysts that can treat various contaminant properties across various media, there have been encouraging developments in heterogeneous catalysis. Alterations to conventional reactors can exaggerate existing processes and chemicals, and adding additional steps to the reactor can increase catalytic activity.

4.2. Resource Recovery and Desalination.

The desalination problem requires a pressing need to increase energy efficiency and valorise by-products. Today, the situation in desalination underscores the need to reduce electricity use and mitigate environmental degradation (Wang et al., 2023). In its current form, reverse osmosis (RO), which has been considered a sustainable approach, continues to require substantial energy and produces waste brine, raising the question of whether to dispose of it or reuse it. Instead of considering only the brine waste stream, hybrid desalination systems and methods that transform brine into marketable products are economically motivated (Lee et al., 2019). In the meantime, new materials are required to develop low-energy desalination processes and restructure the desalination process into a continuous structure. These innovations can enable greater energy reuse in desalination and the development of hybrid solutions that enhance brine removal or offer alternative approaches to recover and generate disinfectants.

4.3. Wastewater Valorisation

The chemical pathways for wastewater valorisation aim to upcycle into higher-value products that meet market demand, generate revenues and jobs, and therefore provide value addition that compensates for treatment costs. Natural organic matter sources are excellent sources of carbon in the form of amino acids, proteins, and carbohydrates, which are used to produce compounds with biological, pharmaceutical, and agricultural uses. Untreated wastewater may be converted into a useful biopesticide using urea. Plastic trash and wastewater may be jointly treated to generate organic acids through a joint-commodity approach. Coffee pulp-fermented liquor can serve as a carbon and nitrogen source to support microbial growth and to produce polysaccharides. During the last decade, there has been a move towards the acquisition of biochar, platforms, and oils with an H/C ratio of 700 1.4 from raw and fortified wastewater sludge, due to the proximity of nutrient-rich sludge to consumers, the generation of energy and the recycling of nutrients.

The idea of converting organic contaminant content into water resources and the value placed on water resources are compatible with the concept of the circular economy. This type of innovation can modernise current treatment plants in the food and beverage sectors with high organic loading at a low investment cost, thereby enabling on-site valorisation and upcycling rather than remote treatment or loss of agronomic or economic value. Without energy input or the use of waste-derived substrates, wastewater containing target ingredients with application value can be transformed to support the in situ growth of bioproducing organisms.

Table 2. Water technologies and wastewater valorisation

Approach/technology	**Target problem**	**Key mechanism/process**	**Potential co-products/value streams**	**Major challenges/trade-offs**
Advanced water treatment catalysis (AOP, etc.)	Micropollutants, complex contaminants	Photocatalysis, electrocatalysis, redox reactions	Decontaminated water, possible recovery of specific species	Catalyst robustness, energy input, and multimedia handling
Desalination (RO and hybrid systems)	Freshwater scarcity	Membrane separation, hybrid thermochemical steps	Freshwater supply, mineral recovery from brine	High energy demand, brine disposal vs valorisation
Brine valorisation and hybrid desalination	Brine waste from RO	Coupled separation and conversion routes	Industrial salts, chemicals, disinfectants	Process complexity, market for by-products
Wastewater-to-biochar/oils	Organic-rich	Thermochemical conversion	Biochar, platform	Product quality control,

Approach/technology	Target problem	Key mechanism/process	Potential co-products/value streams	Major challenges/trade-offs
	wastewater, sludge	(pyrolysis, etc.)	oils, energy recovery	emissions, scale-up
Integrated plastic–wastewater treatment	Plastic waste plus organic wastewater	Combined degradation and bioprocessing	Organic acids, useful intermediates	Process integration, feed variability

5. Environmental Protection and Remediation.

Human survival depends on access to sufficient clean energy, water, and air. However, the chemical interventions that have made such resources available have, unfortunately, placed significant burdens on supporting ecosystems. The need to curb these undesirable outcomes has been the theme of environmental protection.

Sustainability frameworks point to the necessity of creating more useful chemical products from less, less impactful materials, with lower emissions and fewer toxic, harmful, and pollutant properties (A. Burke et al., 2017). Concurrently, the defence against ecological degradation may take the form of remediation, restoration, creation, or conservation. It is often not possible to restore balance without human involvement; therefore, the complementary chemical techniques have become commensurate with the mitigation measures.

5.1. Green Catalysis to Abate Pollution.

Oxidising and reducing catalysts will help reduce environmental pollution and limit the consequences of climate change. The new green catalysts have also been found to be much more efficient and stable than the catalysts used previously. A wide range of precursors, supports, and dopants have been used in these materials, which allow for a range of relevant and varied reaction pathways for the breakdown of air and water pollutants and relax the conversion of greenhouse gas emissions (e.g., H_2S, CO, CO_2, and methane), thereby producing fewer harmful by-products. Waste, metal-organic frameworks, biomass, and zeolites are some materials that play a major role in the degradation of plastic waste. Also, the development of catalysts that can oxidise hydrochlorofluorocarbons in the stratosphere is one of the most important measures to curb ozone depletion. After minimising harmful substances, focus on reducing hazardous emissions during the AOT process. In this respect, photocatalysts offer new opportunities, yet their efficiency and stability should be improved.

The anthropogenic emissions of environmental pollutants into the atmosphere, land, and water require special attention and catalysts to mitigate their harmful effects. These materials are clustered into two broad categories: green catalysts for the oxidation/reduction of hazardous materials and those of AOT, where more and more materials are based on alternative precursors to the traditionally used noble metals. A broader range of reaction pathways is now amenable to a variety of precursors, supports, and dopants, opening up opportunities to tap new mineral and clay stocks. Of interest in the prevention of ozone layer depletion is the incorporation of metal and zeolite clusters into the oxidation of hydrochlorofluorocarbons in the stratosphere. It has also developed photocatalytic materials for advanced oxidation processes. However, their practical use needs to be improved, particularly in terms of efficiency and stability, including their ability to operate under real atmospheric conditions.

5.2. Waste Minimisation and Circular Economy.

The movement towards a Circular Economy (CE) aims to sustain the value of materials and products as long as this is technically feasible, and hence to reduce their degradation into waste and to be part of sustainability. This aspiration is embodied in several material-use strategies (Aristi Capetillo et al., 2022), thus the extension of cycling, flows in-use, and Platform Development, which do not, in turn, become waste themselves. A mature industry has complete preparedness at any phase in the evolution of excess production of all materials equal to or more than the nominal manufacturing wastes, in all the successive economic-material or process-energy processes.

Used or overspent chemicals are recycled through successive use cycles before being disposed of as waste. Circular strategies are directed towards the performance of cease or sustain hold of long-out-of-public-use flows in the acquisition and delivery of virgin-use energy or materials. A simple organisation of products and pro-circulation re-entry reinforcement fosters value stability and in-use prolongation of co-products, and, in all flows, helps transfer back to the same reacquirable material initially extracted or otherwise utilised. Development of disassembly-friendly packaging makes it easier to reduce end-of-life degradation in the pre-consumer cycle and to renew chemical supplies.

5.3. Life Cycle Assessment and Impact on the Environment.

Life cycle assessment (LCA) is a systematic tool for quantifying the environmental effects of chemical processes over their life cycle, including resource extraction and production, process operation, utilisation, and finally disposal or recycling. The following are the main modules of the LCA framework:

(1) definition of study goal and scope,

(2) inventory analysis,

(3) impact assessment and

(4) interpretation.

The former module identifies how the study is to be used, the intended audience of the study report, and the role of the chemical product or process under analysis. The functional unit is determined to normalise outcomes across production scales and to enable comparison of processes; it is the volume of the product or service that represents the process's interest. The other attributes that can be included in a goal-and-scope statement are system limits (e.g., cradle-to-gate, cradle-to-grave), the process under investigation, emission and resource-use targets, and limitations of the LCA model (e.g., geographic or technological).

The second module is the inventory analysis, which entails quantifying all resource inputs (e.g., energy, water, chemicals) and waste outputs (gases, liquids, solids) of the technology in question. Various data sources could be used. Primary data is preferred, although secondary data, including material or environmental flow data of the corporate sustainability reports, online databases, or published research, is usually necessary. The main source of primary data is previous research reports that have used LCA to assess the environmental consequences of chemical processes, such as alternative technologies, process intensification, and the communication of sustainability measures. Based on this inventory data, the environmental effects of the process across its life cycle are measurable using commercial software and library databases for LCA.

6. Integrated System Design and Modelling.

The growing demand for energy, water, and raw materials is becoming a major concern for the sustainability of existing production and consumption trends. Currently, complex energy-water-environment systems are under intense research due to their inevitable interdependencies and resource scarcity. A more interdisciplinary design approach is required to capture the system's interdependencies and investigate new directions for the energy switch (da Costa Junior et al., 2018). Integrated design is achieved by specifying the system boundaries, defining contextual constraints, tracing functional units, estimating key performance indicators quantitatively, and evaluating all possible interactions (Qin, 2007).

Large-scale chemical operations are usually limited by operational, performance, and sustainability objectives that must be met within a particular design. To cater to such varied requirements, modelling capabilities that support system and process modelling, with an emphasis on rigorous simulation/optimisation, and data analysis, are currently available. The current global trend toward stricter environmental regulations has become a serious driver of chemical processes that reduce energy use, emissions, waste generation, distribution, and the use and consumption of hazardous substances. In this regard, predictive tools and sustainability assessment strategies are the most important for realising the interdependencies between the constraints of governed systems and the associated sustainability measures across the entire life cycle of chemical or process technologies. A wide range of modelling methods for assessing sustainability, along with ancillary methods for creating a viable and sound modelling framework, is introduced. The ways of decision-making that can be used to ensure that paths are taken to guarantee compliance with environmental regulations without affecting the overall economic performance of the chemical industry worldwide emerge as a category of high interest.

6.1. Coupled Energy-Water-Environment Systems.

Energy, water, and environmental systems are inherently interconnected and often exhibit synergistic interactions. As an example, energy supply systems and technologies that generate fresh water through seawater desalination or water treatment can, in principle, be located in the same place and complement each other during crises (e.g., droughts or floods). The shared resource of freshwater may, however, be subject to competition when the amount of energy or chemical processes consumes much of the water that the water production facility can produce. Scarcity of water may also result in fewer energy supply and storage facilities within a region, leaving it susceptible to systemic shocks. These interdependencies are critical when the supplying or consuming technologies/systems are inefficient or unsustainable.

One way the interconnectedness of these resources is demonstrated is through the chemistry of sulfur and its numerous forms, which can play a significant role in connecting energy, water, and the environment. Resource-use flows and diagrams are becoming increasingly popular for elucidating interdependencies and trade-offs within energy-water-environment interactions, particularly in specific regions or for specific technologies. Coupled Energy-Water-Environment (EWE) systems diagrams provide a graphic overview of integrated flows of resource use across the interrelated subsystems of energy, water, and the environment, and show how process-level gains in the individual subsystems can alleviate energy-water-environment trade-offs and enhance resource availability among the systems.

6.2. Sustainable Process Design Modelling Tools.

Sustainable process design is the process of choosing the routes of chemical production that reduce adverse environmental effects and preserve the economy and safety. Process design in chemical engineering usually involves modelling material and energy flows and specifying reactor and separation units. This mainstream activity is complemented by sustainability-based techniques, including a chemical process simulator for flowsheet simulation and a spreadsheet tool for sustainability evaluation (Ibrahim Samli, 2011). The other method is the coupling of process design and Life Cycle Assessment (LCA) to systematically identify changes that reduce environmental and economic footprints (Fernando Morales-Mendoza et al., 2018). The solution to the problem of water scarcity or pollution must be approached in the same integrative, systemic manner as with energy technologies.

6.3. Making decisions in situations of Uncertainty.

Chemical technologies should undergo constant evolution to ensure that the world has long-term, sustainable solutions to energy, water, and environmental challenges. The nature of these technologies is characterised by trade-offs since a solution to one problem developed as sustainable is likely to lead to a new problem or requirement on another. Sustainability evaluation also raises significant doubts about the long development times required for chemical processes. In view of these complexities, there is a need for strong, resilient solutions that not only meet technical requirements and economic viability but also operate satisfactorily within sensitive chemical and energy infrastructures and the uncertainties arising from larger environmental and economic forces.

In clean, efficient, safe, and sustainable chemical engineering, chemical technological innovation is pursued through a systems approach. To start with, sustainable chemical technologies should be developed within an overall approach to energy, water, and environmental problems, since these issues are interconnected in the global systems of energy-water-environment-food-economy. Second, the systemic views of the system, which are interdependency, synergy, and trade-off between materials, infrastructures and processes, and energy distribution, must be taken into account during the development of sustainable chemical technology since a sustainable attitude in one field is often accompanied by contradictory developments at the other. Specific systems analysis involves the analysis of coupled chemical infrastructures, including energy-water-environment and food-water-energy structures, involving bioprocessing. Third, a decision must be made amid uncertainty when developing a sustainable chemical process. Systems thinking sheds light on the boundaries, feedback loops, leverage points, and interdependency of processes and infrastructure, hence enabling different viable paths and options to be discovered in addition to aiming at a broader set of environmental, economic, and social indicators of sustainability subject to unpredictable changes and conflicts of the long term (Yue Nina Chen, 2005). There are well-defined uncertainties throughout the development route, as well as more extensive environmental and economic factors and associated risks, all of which are subject to stringent evaluation. Further checks and scenario analysis are offered by robustness and sensitivity tests (A. Bras & Paredis, 2006). The modelling framework, tools and illustrative examples promote insights into the characterisation and quantification of uncertainty, risk estimation and multi-dimensional strong checks in economic, environmental and social sustainability under interrelated and integrated circumstances.

7. Policy, Regulation, and Governance.

Modern life is unimaginable without chemicals, which underpin modern materials, from agriculture to pharmaceuticals. Nonetheless, the physical and sociocultural harm caused by conventional chemical processes screams out for sustainability. In turn, the focus of research efforts on means to facilitate the shift to sustainable energy, water, and environmentally friendly materials has been on chemical technologies, particularly catalysis and electrocatalysis. However, that is not enough innovation. Tubular change necessitates supporting systems that facilitate process modification in response to fluctuations in supply and demand, prices, and regulations. Notably, sustainability challenges extend beyond chemical transformation and include broader issues of consumer behaviour, governance, and regulations (P. Wilson & R. Schwarzman, 2009): consumers prioritise accessibility over sustainability, sustainability concerns subside after purchase, and capital investment and incentive regulation do not reflect sustainability performance. This is an incredibly complex challenge that demands a similarly complex systems perspective so that one can recognise the problem's boundaries and the influence it has on other changes, which would either support or weaken the intended course.

Sustainability is necessarily related to chemical processes. This fact not only provides the scope of chemical sustainability itself but also of the policy, regulation and governance of chemical technologies. These mechanisms have the potential to make the process of change more radical, guide the direction one wants to go, and reduce a rebound effect in which innovation leads to a return to previous practices.

7.1. Standards, Incentives and Compliance.

Pollution and waste from chemical processes and materials are enormous, and resources are being exhausted. Process and material sustainability have become major issues in the chemical industry, which is under ever-increasing pressure to minimise its environmental impact. The reduction of the chemical sector's ecological footprint can be significantly achieved through pollution and waste prevention methods. A circular economy solution is required to meet high environmental standards and maintain industry competitiveness. Sustainability awareness and waste legislation have led to a shift in emphasis from process LCA to product life-cycle assessment (LCA). The most widespread approach to introducing sustainable chemical technologies is regulation. Governments have established standards and regulations on emissions to limit emissions to acceptable levels. Regulatory forces, on the other hand, are creating an increasing incentive for the use of green technologies, which centres on products. Prescriptive regulations are procedures, performance levels, and technologies that must be met. In contrast, other adaptive mechanisms are outcome-oriented, e.g., through taxes, damaging fees, or tradable credits, to achieve innovative alternatives towards broader targets.

There are barriers to accessing or distributing sustainable technologies, including a lack of clear definitions and supporting measures for researchers and decision-makers, the interdisciplinary pull on researchers and managers, and the misalignment between professional incentives and sustainability goals (Jen Mendelsohn Matus et al., 2013). The most important in setting the performance criteria in tangential areas of regulation is the chemical industry and process engineering. The possibility of offering systematic assessments of product/process sustainability, as well as mere decision heuristics, to client firms is a potentially fruitful point of intervention. New formal methodologies are needed to encourage quantitative exploitation of potentially large numbers of chemicals or classes of substrates. Energy-water-environment technologies and performance thresholds should be analysed in a standardised way, enabling the qualitative variables to be compared across different documents and between processes (Ibrahim Samli, 2011).

7.2. Ethics and Responsible Innovation.

Responsible innovation frameworks should guide the development of sustainable chemical technologies to address society's needs broadly. The frameworks facilitate innovative practices that align with the aspirations, desires, values, and ethics of people in society. The stakeholders' input would be expressed as expectations, requirements, and the technology's preparedness; two-way communication would help build pre-existing and ongoing social acceptance. Social license to operate is further enhanced by academic and industrial advancements towards socially desirable outcomes, such as a just, equitable and prosperous society, environmental integrity and economic viability. Such anticipatory ethics as precaution, reversibility, and justice are used to maximise the positive outcomes and minimise the negative effects. The practice of socially constructive conversations fosters trust in society. Involvement in society devises novel governance tactics that emulate the practical and symbolic achievements of renewable energy technology implementation.

The precautionary principles help prevent the engineering of disasters, and Roberts presents questions to support responsible chemical research, including: Will field testing of the new molecule alarm people about remote-area disease-control products? Are the newly invented pesticides safe to non-target organisms? Will the chemical industry be strong enough to withstand the people's criticism? Will there be more unemployment in the chemical industries? Who will benefit most? Are the regulatory authorities and their funds adequately prepared to expand to meet the industry's needs? Can missionary groups co-exist with the chemical industry? Any new engineering technology project should strike a balance between the freedom to create societies and the need for fair reversibility and controllability in case of failure. Cautious foresight of the global risks of every new technology may enable chemically predetermined fine systems to address previously insoluble global issues.

8. Sustainable Chemical Technologies Case Studies.

Sustainability is being viewed as a need rather than a goal (Ibrahim Samli, 2011). The chemical industry has contributed to environmental pollution. Technologies are thus being developed to provide clean energy, clean water, and clean air, thereby enhancing human health and safeguarding biodiversity. However, these sustainable chemical technologies are not perceived as an integrated system but instead taken separately (Adalja & U-tapao, 2013).

8.1. Green Hydrogen Supply Chains Case Study.

Hydrogen has been described as the cleanest energy carrier, with zero emissions at the point of use. Manufacturing green hydrogen through electrolysis and using renewable energy helps reduce GHG emissions during production. Hydrogen can store energy for long periods and has a high energy density, making it a viable alternative to current batteries. Hydrogen gas can be transported via pipelines and tankers, thereby serving a larger supply area. However, the broad implementation of hydrogen supply chains is not possible due to various issues: hydrogen is difficult to transport; it is difficult to store; liquefaction is an energy-intensive process required to transport it in large volumes; and its use is limited by safety concerns (Eu Chew et al., 2023).

It is expected that hydrogen will be used in industry and mobility. A systems view is thus required to identify synergies and trade-offs in the hydrogen supply chain, understand interactions with other systems, and investigate interactions with other energy carriers and conversion technologies (Liang, 2010).

8.2. Case Study: Catalytic Water Treatment and Advanced Oxidation.

The use of highly sophisticated oxidation processes (AOPs) as an alternative treatment for water has been driven by rapid technological and environmental change worldwide. The AOPs are used in pharmaceutical micropollutants, biorecalcitrant organic matter, and new contaminants, including endocrine-disrupting compounds. Besides enhancing catalytic activity, recent research has focused on catalyst stability to increase practical applicability and extend their lifespan, thereby reducing contaminant generation associated with them. Among a range of processes, semiconductor AOP photocatalysis has become widely industrialised for organic indoor air treatment and aerosol disinfectant atomization, which recently received a new push due to the COVID-19 pandemic. In semiconductor photocatalysis, titanium dioxide is the most widely used photocatalyst worldwide, although durable alternatives are becoming increasingly popular. Nanomaterials Two-dimensional (non-metallic) catalysts (like graphene oxide, phosphorene, tungsten diselenide and hexagonal boron nitride) are also potential catalysts of catalytic oxidation, including low-temperature combustion of methane, which is a major world security issue. Advanced oxidation processes: Catalytic oxidative AOPs and electrochemical AOPs have emerged as complements to semiconductor AOP photocatalysis. Vinyl acetate polymerisation, aided by catalysts and low-temperature carbon monoxide oxidation, has remained of great academic interest.

Although both advanced oxidation and catalytic processes are energetic and effective for treating water, wastewater, and atmospheric fluids, they also tend to produce internal pollutants, including acids, metallic compounds, and organics. It is important to tackle the energy production vs. pollution trade-off in order to preserve the hydrospheric, biospheric, and atmospheric commons of the world (Antonio Garrido-Cardenas et al., 2019; Udom, 2014).

8.3. Case Study: by-products valorisation Industrial by-products.

Economic models posit that the supply of minerals such as phosphorus, molybdenum, and cobalt will be critical in the next few decades (Rachel Lombardi et al., 2012). In 2011, the United Nations sounded the alarm over possible shortages of phosphorus, which is crucial for food security. The reserves of phosphorus can be as little as 100 years. In addition, the chemical industry uses more than 2.5 trillion litres of water each year (Summerton et al., 2019). Waste products, such as industrial by-products, can be valorised to isolate useful products, resulting in economic gain. The examples include the extraction of minerals such as phosphates and sulphates, and the isolation of rare earth metals from seawater, produced waters, and industrial discharges. This has been developed using approaches such as direct extraction, selective adsorption, precipitation paths, and (bio)catalytic processes. The multidisciplinary framework simulated strategic investment in these technologies, taking into consideration aspects such as hazardousness, valorisation potential, and uncertainty to identify a sustainable opportunity. The upcycling of related by-products in gasification or biomass streams was also made clear by systems analysis, which enabled synergetic valorisation, thereby increasing the range of products sold in the marketplace. Material- and energy-intensiveness were also calculated across a wide range of valorisation and upcycling options to put them in economic perspective.

9. Gaps in Knowledge and Horizons of Research.

Currently, water, energy, and environmental problems are among the most urgent issues in people's lives. The solutions to these challenges, as well as the development of new technologies and innovative products in the future, are centred on chemicals and chemical reactions. Chemical processes have been studied in depth to ensure sustainability. Nevertheless, this body of work remains fragmented, and high-impact progress is frequently neglected. A systems thinking approach is necessary to enable profitable and responsible chemical innovations, taking into account system boundaries and feedback across the various desirable sustainability goals. However, there is less research on the principles of systems thinking, frameworks, and methods of sustainable chemical technology.

This part identifies knowledge gaps and research frontiers with significant impact on sustainable chemical technologies and systems thinking. The proposed list of 26 research questions is intended to influence academic interest in chemical technologies for sustainability and to promote a more systems-focused approach. Top priority questions include integrated energy-water-environment systems, governance outside the chemical sector, and the discussion of new relations between products and processes enabled by digitalisation (A. Burke et al., 2017; Schlögl, 2016). These questions would be considered, and the systems thinking and the development of sustainable chemical technologies would be improved.

10. Conclusion

Sustainable chemical technologies integrated into renewable energy cycles, water quality and supply, and the environment contribute to social prosperity and economic resilience. A systematic review is a source that determines configuration options, moderate system responses, and elucidates implications of sustainability. Alternative energy futures are integrating circularity, multiple energy carriers, and industrial bioprocessing into chemical and material supply chains.

Water purification has characteristic features of integrated water-energy systems, including advanced oxidation for pollutant oxidation, electrochemical resource removal from wastewater, and closed-loop recovery of resources as biogas in brownfields. Improved capture in air-gas-phase treatment, the circular economy with product lifetimes, multilevel reporting of the life cycle, and changes in regimes in energy-chemicals systems map the prospects for systematic development. The extensive implementation depends on policy frameworks that facilitate stakeholder involvement, set safe design criteria, apply an equity test, and secure a social license to operate.

Systemic interaction should be considered to supplement sectoral perspectives, improve the identification of leverage points towards sustainability, and ensure sufficient regulatory focus. The systems-driven research directions include coupled resource systems, uncertainty-driven design and decision-making, and the interaction of technology and governance. There is a need to put in more effort to advance the emerging systems-software ecosystem toward achieving simultaneous process-product portfolio specification and performance prediction.

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