

Review

# Process Design and Sustainable Development

Peter Glavič<sup>1,\*</sup>, Zorka Novak Pintarič<sup>2</sup> and Miloš Bogataj<sup>3</sup>

<sup>1</sup> Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, SI-2000 Maribor, Slovenia; peter.glavic@um.si

<sup>2</sup> Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, SI-2000 Maribor, Slovenia; zorka.novak@um.si

<sup>3</sup> Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, SI-2000 Maribor, Slovenia; milos.bogataj@um.si

\* Correspondence: peter.glavic@um.si;

**Abstract:** This review paper describes some historical facts, the state of the art of process design and sustainable development. In the Introduction the most important global megatrends are presented and the European Union response to them, the European Green Deal. Process design and sustainable development are dealt with separately and holistically. Organization of professionals from the area, their conferences and publication are supporting the two topics. A short analysis of the published documents in two most popular databases shows that environmental dimension is prevailing, followed by economic one while social pillar of sustainable development is undervalued. The most important design tools for sustainability are described. An important practical case, the European chemical and process industries are analyzed and their achievements in sustainable development are shown; in particular their strategies are presented in more detail. The conclusions are embracing the most urgent future development areas of process industries, carbon capture with utilization or storage, the process analysis, simulation, synthesis and optimization tools; zero waste, circular economy and resource efficiency are already playing an important role. But deeper changes are needed in the future decades including de-growth with changes of habits, lifestyles, and business models. Lifelong education for sustainable development will play a very important role in the growth of democracy and happiness instead of the consumerism and neoliberalism.

**Keywords:** process design, sustainable development, chemical industry, process industry, megatrends, design tools

## 1. Introduction

In the Introduction some basic information about process design and about sustainable development will be presented, separately for both of them as well as together. Then we shall proceed with the up to date results and finish by conclusions. But before going into details we are going to look at the global megatrends of future development which are speculating about our fate: "Trends are an emerging pattern of change likely to impact how we live and work. Megatrends are large, social, economic, political, environmental, or technological changes that are slow to form, but once in place can influence a wide range of activities, processes, and perceptions, possibly for decades. They are the underlying forces that drive change in global markets, and our everyday lives [1].« Although megatrends are not deterministic, they can help us in planning and developing products, processes and services for the future customers. Many studies on megatrends are available [2–4]. Six megatrends and their implications are shown as an overview of them:

1. **Climate change** – a) Air pollution with GHGs, b) Exponential climate impacts (extreme weather events, air-land-oceans heating, polar ice caps, permafrost and glaciers melting, sea level rise, wild fires, deforestation and deserts), c) Loss of biodiversity and ecosystem services; Implications: i) Decarbonization, reforestation, green buildings, carbon capture with utilization or storage, ii) Tax on GHGs emissions, iii) Beyond GDP metrics.

2. **Resource scarcity** – a) Increased strain on the planet's resources including a degraded soil, b) Food-water-energy nexus, c) Critical raw materials; Implications: i) Zero waste, circular economy and increased efficiency, ii) Shift from fossil fuels to renewable energy and bio-based raw materials, iii) Microbiomes (bacteria, archaea, fungi, viruses and nanoplankton), synthetic biology (intersection of biology and technology).
3. **Shifting economic power** – a) Emerging economies (E7) as the growth markets, b) Global demographics change (different population growth rates), c) Techno-economic cold war; Implications: i) Power shift from west (G7) to east (E7), ii) Industry 4.0 (the fourth industrial revolution, use of cyber-physical systems), iii) Consumer preferences are changing, e.g. in the food industry (organic and fresh food, online delivery).
4. **Technological breakthrough** – a) The pace of change is exponential, not linear, b) Data is the new oil, c) Automation and robotization (many jobs will be replaced by machines/robots); Implications: i) Digitalization – AI (Artificial Intelligence), big data, 3D printing, 5G network, IOT (Internet of Things, 26 billion 'things' are connected by internet), ii) Increased research and innovation, iii) Industry 5.0 (interaction of human intelligence and cognitive computing).
5. **Demographic and social changes** – a) Population continues to grow, b) More old people and fewer children, c) Income inequality rise; Implications: i) Healthcare spending (rise of expenses, saving for retirement), ii) Education for sustainable development, lifelong learning, creativity, entrepreneurship, iii) Higher taxation of high incomes and succession duties.
6. **Rapid urbanization** – a) Migration to the cities (mega cities), b) Life is better in the cities; Implications: i) Smart cities, new infrastructure, ii) Healthcare and security (changing disease burdens and risk of pandemics, crimes and terror – surveillance, monitoring), iii) Consumer behaviors change (resources will be shared, move from energy suppliers to mobility solutions).

Special studies exploring the future trends in different areas exist. Let us mention one of them – New Energy Outlook (NEO) [5]. It has three major parts: 1) Economic Transition Scenario (ETS), 2) NEO Climate Scenario (NCS), and 3) Implications for Policy. The Executive Summary has six chapters, each one with several scenarios: a) Energy and emissions, b) Power, c) Transport (general, road, shipping, aviation, rail), d) Buildings, e) Industry, and f) Climate.

Industry consumes 29 % of total final energy. Energy consumption grows at an average of 0.6 %/a (per year), reaching 149 EJ (exajoules, 10<sup>18</sup> J) by 2050. Steel and chemicals are the two largest energy consumers in industry, responsible for 19 % and 18 % of final energy use in the sector in 2019. They are followed by cement, at 14 %, and aluminum, at 6 %. Around 12 % of all fossil fuels consumed in industry are used as a feedstock for non-energy purposes (from petrochemicals to plastics). In 2050, the sector will account for around 34 % of emissions from fuel combustion, up from 25 % in 2019. Energy demand for steel will grow 50 %, for aluminum 80 % and for plastics 100 %. High investments in energy – wind 3.3 T\$ (trillion US dollars = 10<sup>12</sup> \$) and solar 2.8 T\$ – are expected by 2050. Prices of renewable wind and solar energy are forecast to fall by about 50 % [6].

### 1.1 European Green Deal

Climate change and environmental degradation are an existential threat to Europe and the world. European Commission responded to some of the risks mentioned in the Megatrends with the Green Deal. It aims to transform the Union into a modern, resource-efficient and competitive economy where:

- There are no net emissions of greenhouse gases by 2050;
- Economic growth is decoupled from resource use;
- No person and no place are left behind [7].

European Green Deal (EGD) will have a deep influence on life in European Union, both on personal and on enterprise levels. It will also very deeply hit the chemical and process industries.

EU has met its GHG emissions reduction target for 2020, and has put forward a plan to further cut emissions by at least 55 % by 2030. By 2050, Europe aims to become the world's first climate-neutral continent. Climate action is at the heart of the European Green Deal – an ambitious package of measures ranging from ambitiously cutting greenhouse gas emissions, to investing in

cutting-edge research and innovation, to preserving Europe's natural environment. Its action plan aims to:

- Boost the efficient use of resources by moving to a clean, circular economy;
- Restore biodiversity and cut pollution.

One of the first activities is the European Commission's proposal of the European Climate Law, a legally binding target of net zero greenhouse gas emissions by 2050. A system for monitoring progress and take further action if needed is planned. Reaching this target will require action by all sectors of the economy, including:

- Investing in environmentally friendly technologies,
- Supporting industry to innovate,
- Rolling out cleaner, cheaper, and healthier forms of private and public transport,
- Decarbonizing the energy sector,
- Ensuring buildings are more energy efficient,
- Working with international partners to improve global environmental standards.

EGD and a European COVID-19 response can address Europe's climate, biodiversity, pollution, economic, political and health crises, and at the same time strengthen its institutions and reignite popular support for the European project. SYSTEMIQ and The Club of Rome published a report A System Change Compass concentrating on the drivers and pressures that lead to these environmental challenges and on solutions and required changes to the current economic operating model [8]. The report: a) foresees radical resource decoupling and sustainability, b) offers a system perspective, c) starts from the human drivers for change, d) offers a set of principles for support, e) it takes natural system as a starting point. To achieve this system-level change, the report addresses three fundamental barriers for the change: 1) shared policy orientations at the overall system level, 2) systemic orientation for each economic ecosystem, and 3) a shared target picture and roadmap for Europe's next industrial backbone.

The System Change Compass offers:

- Each of the 10 principles has 3 orientations giving 30 system-level political orientations for the overarching system as a checklist for policymakers;
- 8 ecosystem and 3–5 ecosystem orientations (directions) for Europe's industrial backbone;
- Over 50 Champion orientations (directives) that form a view of industrial priorities.

The 10 principles with their orientations are including the following redefinitions:

1. Prosperity – from economic growth to fair and social economics;
2. Natural resources - consumption and development decoupled, a shift to responsible usage;
3. Progress – from economic activities/sectors to societal needs within planetary boundaries;
4. Metrics – from GDP growth to natural capital and social indicators;
5. Competitiveness –EU based on low-carbon products, services and digital optimization;
6. Incentives – aligned with the Green Deal ambitions and economic ecosystems;
7. Consumption – from individual identity to individual, shared and collective identity;
8. Finance – from subsidizing 'old' industries to supporting economic ecosystems;
9. Governance – from top-down to transparent, flexible, inclusive participatory one;
10. Leadership – from traditional to system one, based on and intergenerational agreement.

The eight economic ecosystems with over 50 Champions are resulting in industrial priorities:

1. Healthy food (organic, no waste, water, urban agriculture, alternative proteins, etc.);
2. Built environment (planning, ownership, buildings repurpose and retrofit, net zero, circular);
3. Intermodal mobility (high-speed railways, green aviation and shipping, ride sharing, etc.);
4. Consumer goods (product-service, product sharing, maintenance and value retention);
5. Nature-based (degraded land restoration, urban greening, ecotourism, paid ecosystem services, forest, sea, marine and land protection);
6. Energy (renewables, hydrogen, low-carbon fuels, smart metering, carbon capture, grids);
7. Circular materials (value chain systems, asset recovery and reverse logistics, markets for secondary materials, high-value material recycling, materials-service, 3D printing, etc.);
8. Information and processing (distributed manufacturing, high-speed infrastructure, etc.).

## 1.2 Process Design

Process Design (PD) is the choice and sequencing of processing steps and their interconnections for desired physical and/or chemical transformation of materials [9]. The steps are including several unit operations: reaction, separation, mixing, heating, cooling, pressure change, particle size reduction or enlargement, etc. Today, design is governed by circular economy which requires design for repair, reuse, recovery, refurbishment, restoration, and recycling [10]. Process design is distinct from equipment design, which is closer to the design of unit operations. Process design can be the design of new facilities or it can be the modification or expansion of existing ones. The process design may be split into three basic steps; synthesis, analysis and optimization [11].

Design starts with process synthesis – the choice of technology and combinations of industrial units to achieve goals. First, product purities, yields, and throughput rates shall be defined. Modelling and simulation software are often used by design engineers. Simulations can identify weaknesses in a design and allow engineers to choose better alternatives. However, engineers still rely on heuristics, intuition and experience when designing a process. Human creativity is an important element in complex designs.

Process analysis is usually made up of three steps: solving energy and material balances, sizing and costing the equipment, and evaluating the economic worth, safety, operability, etc. of the chosen flow sheet. Optimization involves both structural optimization of the flow sheet itself as well as optimization of parameters in a given flowsheet. In the former one may alter the equipment used and/or its connections with other equipment. In the later one can change the values of parameters such as temperature and pressure. Parameter optimization is a more advanced stage of theory than process flowsheet optimization. Operating manuals on how to start-up, operate and shut-down the process, and maintain safety conclude the process design.

Several considerations need to be made when designing any chemical process unit beside the above mentioned objectives: constraints (capital cost, available space, health and safety, environmental impact, like effluents, emissions, waste minimization and recycling, energy efficiency, operating and maintenance costs), and other factors like reliability, redundancy, flexibility, variability in feedstock and product. Process design documents include: simple block flow diagrams (BFD, rectangles and lines indicating major material or energy flows, stream compositions, and stream and equipment pressures and temperatures), more complex process flow diagrams (PFD, major unit operations, material and energy balances), piping and instrumentation diagrams (P&ID, piping class, pipe size, valves and process control schemes), and specifications (written design requirements of all major equipment items). Process flowsheeting is the use of computer aids to perform steady-state heat and mass balancing, sizing, and costing calculations for a chemical process.

Working Party of the European Federation of Chemical Engineering (EFCE) on Computer Aided Process Engineering (CAPE) is organizing annual events – the European Symposium on Computer Aided Process Engineering (ESCAPE) in which researchers and practitioners in the area of computer-aided process systems engineering from academia and industry take place. Process engineering focuses on the design, operation, control, optimization and intensification of chemical, physical, and biological processes from a vast range of industries: agriculture, automotive, biotechnical, chemical, food, material development, mining, nuclear, petrochemical, pharmaceutical, and software development. The application of systematic computer-based methods to process engineering is called "process systems engineering". Papers presented at the ESCAPE events are all published in Elsevier publications, the CAPE Proceedings Series *Computer Aided Chemical Engineering* [12].

In United States of America (US), a not-for-profit organization CACHE (Computer Aids for Chemical Engineering) organizes the Foundations of Computer-Aided Process Design (FOCAPD) international conferences, focusing exclusively on the fundamentals and applications of computer-aided design for the process industries. The conference is organized every five years and brings together researchers, educators, and practitioners to identify new challenges and opportunities for process and product design. Papers from the conferences are published by the

Elsevier CAPE Book series as *Proceedings of the International Conference on Foundations of Computer-Aided Process Design*.

### 1.3 Sustainable development

Sustainable development (SD) must meet the needs of the present without compromising the ability of future generations to meet their own needs [13]. The Amsterdam Treaty of European Union (EU) sets out the EU vision for a sustainable development of Europe based on balanced economic growth and price stability, a highly competitive social market economy, aiming at full employment and social progress, and a high level of protection and improvement of the quality of the environment. »Transforming our World: the 2030 Agenda for Sustainable Development« including its 17 Sustainable Development Goals (SDGs) and 169 targets was adopted in 2015 by Heads of State and Government at a special United Nations (UN) summit. The Agenda is a commitment to eradicate poverty and achieve sustainable development by 2030 world-wide.

The Chemical Sector SDG Roadmap is an initiative led by a selection of leading chemical companies and industry associations, convened by the World Business Council for Sustainable Development (WBCSD), to explore, articulate and help realize the potential of the chemical sector to leverage its influence and innovation to contribute to the SDG agenda [14]. Building on the Responsible Care program and other sustainability initiatives, The European Chemical Industry Council (Cefic) and its members have developed a Sustainability Charter and agreed on a roadmap to foster innovation [15]. They focused resources in the four critical areas to progress sustainable development:

- Enabling transition to a low carbon economy;
- Driving resource efficiency across global value chains and their operations;
- Promoting the adoption of circular economy principles to prevent waste, achieve low-carbon economy and enhance resource efficiency;
- Preventing harm to humans and the environment throughout the entire life cycle.

International Conference on Sustainable Development (ICSD) is organized annually by the European Center of Sustainable Development (ECSD) in collaboration with other partners; conference papers are published in the open access European Journal of Sustainable Development, issued by ECSD [16].

The American Institute of Chemical Engineers (AIChE) and the Association of Pacific Rim Universities (APRU, a network of leading universities linking the Americas, Asia, and Australasia) have organized the Conference on Engineering Sustainable Development in December 2019 [17]. They are going to organize the 2<sup>nd</sup> Engineering Sustainable Development Conference in December 2020, both conferences addressing the UN 2030 Agenda for Sustainable Development and the 17 Sustainable Development Goals (SDGs).

Asia Pacific Institute of Science and Engineering (APISE) is organizing International Conferences on Environmental Engineering and Sustainable Development (CEESD) annually; papers are published in the IOP (Institute of Physics) Conference Series: Earth and Environmental Science.

### 1.4 Process Design and Sustainable Development

Process Design and Sustainable Development (PD&SD) started with the ecodesign (ecological design, also called green design or environmentally conscious design) which considered environmental impact of a product throughout its entire life-cycle, only. A typical example is green engineering design [18] which evolved from the green chemistry principles [19]. As sustainable development (SD) has also economic and social components, the additional SD principles have been integrated into engineering design [20]. Today, sustainable development is a part of engineering principles [21, 22].

Crul and Diehl published a handbook on Design for Sustainability (D4S) [23]. Ceschin described the evolution of design for sustainability [24] and Acaroglu overviewed sustainable design strategies [25]. Generic conventional engineering design process is including four phases: 1)



planning and problem definition, 2) conceptual analysis, 3) preliminary design, and 4) detailed design<sup>12</sup>.

Many textbooks on chemical process design are on the market. An older one is dealing with preliminary analysis and evaluation of processes, the analysis using rigorous models, and basic concepts in process synthesis with optimization approaches [26]. Economic evaluation is dealt with, heat and power integration are described to reduce energy consumption, and safety is the only social topic mentioned. In some textbooks, sustainable development, and environmentally sound design (prevent/minimize, recycle/reuse, and recovery) are also described using a few pages [27]. More recent ones are adding steam system and cogeneration, environmental design for atmospheric emissions, water systems, clean process technology as well as inherent safety chapters [28].

Professional literature on PD&SD was more advanced in the past decades as design engineers had to respect laws and regulations regarding environmental protection, labor protection and occupational safety in the approval procedures [29]. Newer literature is including natural resource and environmental challenges, sustainable materials identification, sustainability improvements of engineering designs, evaluation of sustainable designs and monetizing their benefits besides the legislative framework [30]. Sustainability engineering approach is also including Total Quality Management [31] and Life-Cycle Assessment (LCA) [32].

## 2. Process design for sustainability

Publication statistics search in Scopus [33] is including article titles, abstracts and key words. It contains abstract and citation database with over 25,100 titles (articles, conference papers, books, etc.). Searching for the four words: process, design, sustainable, and development yields 16 135 documents, 2 869 of them in open access. There was a constant rise in number of publications since the year 1999 (54 documents), reaching 1859 documents in 2019. By subject area, most of them belong to Engineering (7 060) and Environmental Science (4 090); they are followed by Energy (2 848), Social Sciences (2 777) and Computer Science (2 471). 7 487 of them are articles, 6 330 conference papers, 1 085 reviews, 703 book chapters, and 294 conference reviews. Most of the articles were published in J. Cleaner Production (456), and in Sustainability journal (290). The author with the most publications is R. Gani (39); the most frequent affiliations are Delft University (170), Politecnico di Milano (123), Wageningen University & Research (114), Danmarks Tekniske Universitet (108), and Chinese Academy of Sciences (99). The most frequent keywords are sustainable development (9 604) and sustainability (2 512), followed by design (1 840), product design (1 511), and life cycle (1 514); process design is evidently not so often mentioned.

Similar statistics in the Web of Science (WoS) Core Collection database [34] showed 8 915 documents (14 823 in WoS All Databases); a steady growth was realized in the last four years – from 772 units in 2016 to 1 234 ones in 2019. Most of them (2 557) belong to the categories of environmental science and studies, 1 528 to green sustainable science and technology, 808 to environmental engineering and 620 to energy and fuels. Articles (5 610) are prevailing, followed by proceedings papers (2 700), reviews (818) and book chapters (260). Regarding the organizations, Wageningen University Research (102), Delft University of Technology (98), Centre National de la Recherche Scientifique (89), Helmholtz Association (88) and Chinese Academy of Sciences (86) are on the top.

The WoS Core Collection base covers more than 21 419 journals, books, and conference proceedings while the Web of Science platform includes 34 586 journals, books, proceedings, patents, and data sets. As it was impossible to review several thousand documents, the highly cited ones in the field (121 documents) were selected. Examining their titles lead to 43 documents and by reading their abstracts, 16 articles were selected for a closer look.

### 2.1 Environmental dimension

Most of the 16 articles deal with environmental sustainability, only few of them are including economic dimension, mainly as a criterion for process optimization. Social dimension is seldom present either regarding the workers or the customers or the plant local community. Optimal design

of chemical processes and supply chains is concentrated on energy efficiency, waste and water management [35]. Multiple criteria decision making (MCDM) [36] and Life cycle assessment (LCA) [37] are the tools most often mentioned. Various metrics are used to assess sustainability of processes, e.g.:

- United States Environmental Protection Agency's (EPA) Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator (GREENSCOPE [38]) tool provides scores for the selected indicators in the economic, material efficiency, environmental and energy areas having about 140 indicators in four main areas: material efficiency (26), energy (14), economics (33) and environment (66);
- The Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI 2.0 [39]) for sustainability metrics, life cycle impact assessment, industrial ecology, and process design impact assessment for developing increasingly sustainable products, processes, facilities, companies, and communities it is containing human health criteria-related effects, too; and
- The mass-based green chemistry metrics, extended to the environmental impact of waste, such as LCA, and metrics for assessing the economic viability of products and processes<sup>31</sup>.

Sustainability-oriented innovations (SOIs) in small and medium sized enterprises (SMEs) are integrating ecological and social aspects into products, processes, and organizational structures [40]; the authors are citing five interesting conclusions in their review.

Five out of the 16 articles dealt with biofuels. Purified biogas is an essential source of renewable energy that can act as a substitute for fossil fuels; anaerobic co-digestion is a pragmatic method to resolve the difficulties related to substrate properties and system optimization in single-substrate digestion processes [41]. The synthesis of important biofuels using biomass gasification, key generation pathways for their production, conversion of syngas to transportation fuels together with process design and integration, socio-environmental impacts of biofuel generation, LCA and ethical issues were discussed [42]. A multi-objective possibilistic programming model was used to design a second-generation biodiesel supply chain network under risk; the proposed model minimized the total costs of biodiesel supply chain from feedstock supply to customers besides minimizing the environmental impact [43]. Cultivation, harvesting, and processing of microalgae for second generation biodiesel production, including the design of microalgae production units (photo-bioreactors and open ponds) was described [44]. A multi-objective optimization model based on a mathematical programming formulation for the optimal planning of a biorefinery was developed, considering the optimal selection of feedstock, processing technology, and a set of products [45].

Circular economy topics are the second most numerous ones within the 16 articles. The first one traced the conceptualizations and origins of the Circular Economy (CE), its meanings, explored its antecedents in economics and ecology, and discussed how the CE was operationalized in business and policy [46]; the authors proposed a revised definition of the CE in order to include the social dimension. Another contribution proposed a new unified concept of Circular Integration that combined elements from Process Integration, Industrial Ecology, and Circular Economy into a multi-dimensional, multi-scale approach to minimize resource and energy consumption [47].

High pressure technologies involving sub- and supercritical fluids offer a possibility to obtain new products with special characteristics or to design new processes, which are environmentally friendly and sustainable [48]. Sustainable product-service systems offer service by lending the product to a customer – they attempt to create designs that are sustainable in terms of environmental burden and resource use, whilst developing product concepts as parts of sustainable whole systems that provide a service or function to meet essential needs [49].

## 2.2 Economic and social dimensions

For most managers in industry, economic performance is the most important criterion for decisions on investing money in production and energy facilities [50]. Economic performance indicators are well known, and process and product designs are usually carried out by maximizing

profits or minimizing costs [51]. Other criteria are used less frequently, e.g. the network for the conversion of waste materials into useful products has been optimized using the maximum return on investment [52].

Techno-economic evaluations of process alternatives with different criteria lead in some cases to the same best solution, as Ziyai et al. [53] showed by comparing the three biodiesel production scenarios with the criteria net present value, internal rate of return, payback period, discounted payback period and return on investment. In general, optimization using different economic criteria leads to different optimal process solutions [54]. These processes differ not only in economic performance but also in operational efficiency and environmental impact [55]. This phenomenon is particularly evident in more precise mathematical models [56], which include sufficient trade-offs between investments on one hand and benefits on the other, such as higher conversion, higher product purity, higher degree of heat integration between process streams. Applying the correct economic criteria can lead to more sustainable solutions, for example, the net present value criterion provides optimal process solutions that strike a balance between long-term stable cash flow generation, moderate profitability and moderate environmental impact [57].

With the introduction of the concept of sustainable development, criteria other than economic indicators have become more important in process design, thereby promoting the reduction of negative environmental impacts and the improvement of social performance. When designing sustainable processes, the techno-economic, environmental, and social criteria of various process alternatives are evaluated and the most suitable solution is selected from among them, whereby compromises between all criteria are sought [58]. More systematic approaches use multi-objective optimization. The most common method is to generate equivalent non-dominant Pareto solutions that show a range of solutions where the improvement of one criterion leads to the deterioration of other criteria [59]. However, Pareto curves are not best suited for decision making because the decision maker usually must choose one alternative for realization, which requires additional multi-criteria analyses of Pareto solutions [60].

Another approach is to transform the multi-objective optimization into a single-criterion optimization by monetarizing all pillars of sustainability, which means that in addition to the economic criterion, ecological and social impacts are also expressed in monetary terms. However, this is not an easy task, as environmental and especially social impacts cannot simply be expressed in monetary terms. Environmental impacts are expressed in terms of the burdens and reliefs of the environment. They can be monetized by means of the eco-cost system [61], which expresses the cost of environmental pollution at the price necessary to prevent it. Greenhouse gas emissions can be monetized with a CO<sub>2</sub> tax. Novak Pintarič et al. [62] showed that a deviation from the economic optimum for investments in emission-reducing technologies can lead to a reduction of the tax due to lower emissions, which can compensate for economic loss to a certain extent. The point on the Pareto curve was called the "Economic-Environmental Break Even".

The integration of social effects into process design is difficult and little research has been conducted, although it is becoming increasingly important in both the academic and business environments [63]. The monetization of all the three pillars of sustainable development has been used to synthesize processes and supply networks with sustainability criteria such as sustainable profit [64] and sustainable net present value [65].

Sustainable process designs include various concepts to achieve sustainable solutions; examples are cleaner production [66], zero waste processes [67], zero carbon emission technologies [68], LCA environmental impact assessment in early design phases [69], eco-efficiency indicators [70], etc. Recently, the concept of circular economy has become particularly popular and sometimes even overcomes the term sustainable development, although the terms are by no means equivalent [71]. The concept of circularity is already being used in the design and optimization of technologies and processes, such as the recovery of hydrogen from industrial waste gasses [72] or the development of the novel indicator Plastic Waste Footprint to facilitate an improvement of circularity in the use of plastics [73].

Process systems engineering offers many approaches and tools for the design of process solutions in the field of circular economy and sustainable development, such as synthesis of



processes and supply chains with mathematical programming, process integration, optimization and intensification, multi-objective and multi-level optimization, optimization under uncertainty conditions, etc. [74]. The fact is that circular economy projects, especially those that solve the waste problem, are hardly economically successful on the basis of classic economic criteria, for example, recycling of plastics is not economically viable at low fractions of recycled material [75]. However, it is important to look at these projects in a broader perspective and to include all the three dimensions of sustainable development into design and strategic decision-making.

### 2.3 Process design tools and sustainability

The Process Systems Engineering (PSE) Community has fully embraced the concept of “sustainability” as one of the leading guides in process design. Although it is difficult to pinpoint the exact time when the three pillars of sustainability (i.e. economic, environmental and social) were considered and emphasized simultaneously in the design of chemical processes, one may argue that even the works published as early as late 1970s [76] and early 1980s [77], directly addressed at least two of the pillars of sustainable process design – economic and environmental ones. Although the incentives to develop what we now regard as a sustainable process may have been purely economic at the time, the enabling insight was the ability to view a chemical process as a system – the system that is not isolated from its environment, but a system that interacts with the environment.

Fast-forward five decades of research in the field of PSE, the approaches to designing sustainable chemical processes rely heavily on computer-aided tools. These tools enable simulation, analysis, optimization, and synthesis of chemical processes at various spatial and time scales. From computer aided molecular design [78], simulations of transport phenomena (heat and mass transfer in single or multiphase flows) [79], simulations of single unit operations [80] and whole processes [81] to synthesis and optimization of processes [82, 83] and complete supply networks [84]. The widely accepted approach to assess the sustainability of a given process design is the Life Cycle Sustainability Assessment (LCSA), commonly performed to compare different process design alternatives [85] after the feasible designs have been identified. On the flip side, if a composite sustainability criterion, for example the sustainability profit [86], is incorporated directly into the process synthesis and optimization phase as an objective function, the most sustainable designs can be obtained directly without the need of a posteriori LCSA assessment.

The PSE computational tools enable a practical way to analyze the performance of a wide range of product-process engineering problems as well as to identify the possibilities for improvement. However, some software packages come together with a high license price, and although the price can be justified with the benefits gained, it very often remains an obstacle, especially for small engineering companies. In the last few years, however, the open-source initiatives have begun to offer freely available alternatives to the paid versions (Table 1). Provided that quality matches those of their paid counterparts, greater adaptation of these tools in industry can be expected.

**Table 1:** Licensed and free computational tools, used for process simulation, synthesis/optimization, and sustainability assessment.

Software	Description	Web Site	License
ANSYS Fluent [87]	Computational Fluid Dynamics	www.ansys.com	Licensed
OpenFoam [88]	Computational Fluid Dynamics	www.openfoam.com	Free
Aspen Plus [89]	Process Simulation	www.aspentech.com	Licensed
DWSIM [90]	Process Simulation	dwsim.inforside.com.br	Free
GAMS [91]	Mathematical programming and optimization	www.gams.com	Licensed
PYOMO [92]	Mathematical programming and optimization	www.pyomo.org	Free
GABY [93]	LCA and Sustainability assessment	www.gabi-software.com	Licensed
OpenLCA [94]	LCA and Sustainability	www.openlca.org	Free

## assessment

Identifying what could generally be considered as mitigating solutions to complex problems is necessary, although such solutions may not be sufficient to achieve the goals of sustainable development in the long term. A real breakthrough will be achieved by identifying innovative restorative solutions. In this context, the Process Systems Engineering (PSE) should develop tools that simultaneously address the whole (bio)-chemical supply network. The supply network should be extended for non-diagonal, constitutive elements (nano-robots, molecular machines, labs-on-chips or micro-processes) and linked to other supply networks (energy, agriculture, food, etc.) to form circular and sustainable system-wide supply networks.

Despite many achievements and contributions of the PSE community that undeniably contributed to the development of the modern biochemical and chemical industry, there are no professional tools and hardly any academic ones, specialized in providing innovative solutions to these complex problems.

A noteworthy initiative to develop an advanced computer platform to support innovative conceptual design and process intensification is the IDEAS PSE Framework [95]. The platform addresses the capability gap between state-of-the-art simulation packages and algebraic modelling languages (AMLs) by integrating an extensible, equation-oriented process model library within the open-source Pyomo AML, which addresses challenges in formulating, manipulating, and solving large, complex, structured optimization problems.

The second initiative is MIPSYN-GLOBAL [96]. It is being built on the foundations of its predecessor MIPSYN (Kravanja, 2010), making use of knowledge and experience gained in the decades of research in the field of PSE. The development of MIPSYN-Global encompasses all the four basic PSE tasks: i) development of advanced synthesis concepts, algorithms, and strategies; ii) modeling; iii) development of synthesizer tools; and iv) development of different applications.

### 3. Case study

European Union (EU) is the second largest chemicals producer in the world – with 565 M€ (million euros) it is behind the China (1 198 M€) but before NAFTA (North American Free Trade Agreement – USA and Canada, 530 M€); EU a positive trade balance [97]. About 96 % of all manufactured goods rely on chemistry. Chemical industry is the fourth largest producer after automotive, food and machinery/equipment ones; with the 16 % added value it is the leading sector in EU. 29 000 small, medium, and large companies are offering 1.2 million jobs, 12 % of EU manufacturing employment. Labor productivity in chemicals is 77 % higher than manufacturing average, and salaries are 50 % higher. It is also the largest investor in EU manufacturing. Chemical industry is spending 10 G€/a (billion euros per year) for research and innovation.

#### 3.1 European Chemical Industry Council

The European Chemical Industry Council (Cefic) is the European association for the chemical industry. Cefic developed the Sustainable Development Vision in 2012. It was based on Responsible Care program – a global, voluntary initiative developed autonomously by the chemical industry. It was initiated by the Canadian Chemical Producers' Association – CCPA in 1985, and it is now adopted by almost 90 % of the world chemical industry. Its aim was to improve health, safety, and environmental performance. Cefic's Sustainable Development program started in 2016; it aims at transition towards a safe, resource efficient, circular and low-carbon society. It is organized around the four sustainability focus areas of the Cefic Charter: Create Low Carbon Economy, Conserve Resource Efficiency, Connect Circular Economy and Care for People and Planet [98]:

- Enabling transition to a low carbon economy by:
  - promoting innovation and stimulation of breakthrough technologies development in energy efficient chemicals processes,
  - offering market solutions consistent with low carbon requirements,
  - fostering the development and use of sustainable and renewable raw materials,

- fostering the use of sustainable and renewable energy and raw materials with focus on cost and accessibility,
  - innovating for chemical energy storage
  - developing fuels and building blocks built on CO<sub>2</sub>;
- Driving resource efficiency across global value chains and their operations by:
  - designing sustainable solutions needing fewer resources over the entire life cycle and allowing easy reuse and recycling,
  - maximizing material recovery and reuse,
- Promoting the adoption of circular economy principles to prevent waste, achieve low-carbon economy and enhance resource efficiency;
- Preventing harm to humans and the environment throughout the entire life cycle by
  - mitigating risks, including assessment of substitutes,
  - promoting uptake of safe substances, materials and solutions,
  - minimizing negative environmental impacts on biodiversity and ecosystems,
  - facilitating reuse, recycling, and recovery with steady information flows on products.

In the period 1991–2017 chemical production rose by 84 % while energy consumption was reduced by 16 % and energy intensity by 54 % (–40 % in whole industry) [97]. Fuel and energy consumption was reduced by 24 % in the same period. In the period 1990–2017, Greenhouse gas (GHG) emissions have been reduced by 58 % or 190 Mt/a, from 330 Mt/a down to 160 Mt/a of CO<sub>2</sub> equivalent. GHG emissions per energy consumption have been reduced by 48 % and GHG intensity per production by 76 %. In the period 2007–2017 acidifying emission intensity fell by 40 %, nitrogen emission intensity by 48 %, and non-methane volatile organic compounds intensity by 48 %. These results are typical cases of decoupling economic activity from resource and environmental impacts.

Cefic supported the Green Deal and Europe's ambition to become climate neutral by 2050. In May 2020 the eight-point vision for Europe in 2050 was adopted:

1. The world has become more prosperous and more complex, with a volatile geopolitical environment that brings more economic and political integration within most regions, but more fragmentation between them.
2. Europe has developed its own different but competitive place in the global economy.
3. The European economy has gone circular, recycling all sorts of molecules into new raw materials. The issue of plastic waste in the environment has been tackled.
4. Climate change continues to transform our planet. European society is close to achieving net-zero greenhouse gas emissions while keeping all Europeans citizens and regions on board.
5. Europeans have set the protection of human health and the environment at the center of an uncompromising political agenda.
6. European industry has become more integrated and collaborative in an EU-wide network of power, fuels, steel, chemicals, and waste recycling sectors.
7. Digitalization has completely changed the way people work, communicate, innovate, produce, and consume and brought unprecedented transparency to value chains.
8. The United Nations Sustainable Development Goals are at the core of European business models and have opened business opportunities as market shares increase for those who provide solutions to these challenges.

Cefic has welcomed the European Commission proposal for the European Climate Law turning the climate neutrality objective into legislation and aiming to achieve progress on the global adaptation goal. But besides “what” the EU aims to achieve, the “how” is also important as it will allow the EU to turn this ambition into reality. Cefic puts forward several proposals aiming to clarify, complement or adjust certain provisions by ensuring:

- A sound and detailed definition of climate-neutrality providing a signal for long-term investments;
- A level-playing field for industry across the EU through Union-wide emission reduction mechanisms (i.e. the EU Emissions Trading System, ETS);
- That all sectors of the economy contribute to the climate-neutrality objective through fair burden-sharing;

- Progress on the enabling framework for the transformation of the EU economy, in line with the trajectory for achieving climate-neutrality.

### 3.2 Chemicals Strategy for Sustainability

Cefic calls for a sustainability strategy that recognizes the essential role of chemicals to deliver climate ambitions, and integrates multiple facets of chemicals management including safety, circularity, resource efficiency, environmental footprint, science and innovation. The key components of the strategy should be:

1. Consolidating and promoting the solid foundation Europe has already built, primarily REACH regulation (Registration, Evaluation, Authorization and Restriction of Chemicals), via improvement and better implementation and enforcement;
2. Adopting a proportionate and robust approach for managing emerging, scientifically complex issues;
3. Enabling the development of truly sustainable and competitive European solutions to deliver the Green Deal.

Cefic had welcomed the approach taken by Commissioner Breton to adopt the new Industrial Strategy, basing it on the European industrial ecosystems; actors agreed that the Recovery Plan should be organized around these ecosystems. Chemical processes and products are present in every Industrial Ecosystem in Europe today.

**SusChem** is the European Technology Platform for Sustainable Chemistry. It is a forum that brings together industry, academia, policy makers and the civil society. An important part of SusChem is a network of national platforms (NTPs). SusChem's mission is to initiate and inspire European chemical and biochemical innovation to respond effectively to societal's challenges by providing sustainable solutions. SusChem recognizes three overarching and interconnected challenge areas [99]:

1. Circular economy and resource efficiency – transforming Europe into a more Circular Economy. a) Materials design for durability and/or recyclability, b) Safe by design for chemicals and materials (accounting for circularity), c) Advanced processes for alternative carbon feedstock valorization (waste, biomass, CO/CO<sub>2</sub>), d) Resource efficiency optimization of processes, e) Advanced materials and processes for sustainable water management, f) Advanced materials and processes for the recovery and reuse of critical raw materials and/or their sustainable replacement, g) Industrial symbiosis, h) Alternative business models, i) Digital technologies to increase value chain collaboration, j) informing the consumer and businesses on reuse and recyclability;
2. Low carbon economy – mitigating climate change with Europe becoming carbon neutral: a) Advanced materials for sustainable production of renewable electricity, b) Advanced materials and technologies for renewable energy storage, c) Advanced materials for energy efficiency in transport and buildings, d) Electrification of chemical processes and use of renewable energy sources, e) Increased energy efficiency of process technologies, enabled by digital technologies, f) Energy efficient water treatment, g) Industrial symbiosis via better valorization of energy streams, h) Alternative business models;
3. Protecting environmental and human health – safe by design for materials and chemicals (functionality approach, methodologies, data and tools): a) Improve safety of operations through process design, control and optimization, b) Zero liquid discharge processes, c) Zero waste discharge processes, d) Technologies for reducing GHGs emissions, e) Technologies for reducing industrial emissions, f) Sustainable sourcing of raw materials, g) Increasing transparency of products within value chains through digital technologies, h) Alternative food technologies, i) Novel therapeutics and personalized medicine, j) Sustainable agriculture, forestry and soil health related technologies, k) Biocompatible materials for health applications.

The new SusChem's Strategic Innovation and Research Agenda, SIRA has five chapters:

1. Introduction with an overview where to find the challenge areas;



2. Advanced materials: composites and cellular materials (lightweight, insulation properties), 3-D printable materials, bio-based chemicals and materials, additives, biocompatible and smart materials, materials for electronics, membranes, materials for energy storage (batteries), coating materials and aerogels;
3. Advanced processes (for energy transition and circular economy): new reactor design concepts and equipment, modular production, separation process technologies, new reactor and process design utilizing non-conventional energy forms (plasma, ultrasound, microwave), electrochemical, electro-catalytic, and photo-electrocatalytic processes, power-to-heat (heat pumps, electrical heating technologies), hydrogen production with low-carbon footprint, power-to-chemicals (syngas, methanol, fuel, methane, ammonia), catalysis, industrial biotechnology, waste valorization, advanced water management;
4. Enabling digital technologies: laboratory 4.0 (digital R&D), process analytical technologies (PAT), cognitive plants (real-time process simulation, monitoring, control and optimization, advanced (big) data analytics and artificial intelligence, predictive maintenance, digital support of operators and human-process interfaces, data sharing platforms and data security, coordination and management of connected processes at different levels, and distributed-ledger technologies.
5. Horizontal topics: sustainability assessment innovation, safe by design approach for chemicals and materials, building on education and skills capacity in Europe.

### 3.3 Process industry

**SPIRE** (Sustainable Process Industry through Resource and Energy Efficiency) is the European contractual public-private partnership (cPPP) involving the cement, ceramics, chemicals, engineering, minerals, non-ferrous metals, steel, and water sectors under the Horizon 2020 program. It has been successfully developing breakthrough and key enabling technologies and sharing best practices along all stages of existing value chains to enable a competitive, energy and resource efficient process industry in Europe. SPIRE's new Vision 2050: "Towards the next generation of European Process Industries – Enhancing our cross-sectorial approach in research and innovation" foresees an integrated and digital European Process Industry, delivering new technologies and business models that address climate change and enable a fully circular society in Europe with enhanced competitiveness and impact for jobs and growth [100]. They are contributing 6.3 million jobs in EU. SPIRE community has initiated 77 innovative projects with a total estimated private investment of 3 G€ (billion euros) in the last five years. Their turnover increased by an estimated 25 % – double the EU average.

SPIRE's Vision is that the future of Europe lies in a strongly enhanced cooperation across industries – including SMEs – and across borders to become physically and digitally interconnected. Innovative "industrial ecology" business models will be developed to foster the redesign of the European industrial network. Four "technology drivers" will help the Process Industries achieve their SPIRE ambitions. Two transversal topics – industrial symbiosis and digitalization – will support and accelerate the transformations:

1. Electrification of industrial processes as a pathway towards carbon neutrality: adaptation of industrial processes to the switch towards renewable electricity (e.g. electrochemistry, electric furnaces or kilns, plasma, or microwave technologies).
2. Energy mix and use of hydrogen as an energy carrier and feedstock: renewable electricity, low-carbon fuels, bio-based fuels, waste-derived fuels.
3. Capture and use of CO<sub>2</sub> from industrial exhaust gases (capture, collection, intermediate storage, pre-treatment, feeding and processing technologies, intelligent carbon management).
4. Resource efficiency and flexibility; full re-use, recycling or recovery of waste as alternative resources: collection, sorting, transportation, pre-treatment and feeding technologies; all possible resource streams to be considered and explored (notably plastic waste, metallurgical slags, non-ferrous metals, construction and demolition waste, etc.); zero water discharge, maximal recovery of sensible heat from waste water, substitution of chemical solvents by

water (e.g. in biobased processes); full traceability of value chains as a crucial instrument to deploy circular business models and customers' growing demand for product-related information.

5. Industrial Symbiosis technologies including Industrial-Urban Symbiosis models.
6. Digitalization of process industries has a tremendous potential to dramatically accelerate change in resource management, process control, and in the design and the deployment of disruptive new business models.

The research and innovation efforts of Process Industries under the SPIRE 2050 Vision ultimately want to enhance and – wherever possible – enlarge the underlying value to society generated by their businesses while a) achieving overall carbon neutrality, b) moving towards zero-waste-to-landfill, and c) enhancing the global competitiveness of their sectors.

#### 4. Conclusions

The above mentioned results indicate that the most urgent future development areas of process industries are: climate change with GHGs emissions and ecosystems (terrestrial one is affected by drought, wildfires, floods, glacier melt, or species extinctions; marine one by temperature increases, ocean acidification and sea level rise), energy with renewable sources and efficiency, (critical) raw materials and other resources, water resources and recycling, zero waste and circular economy and resource efficiency, supply chain integration, process design and optimization, process integration and intensification, industrial ecology and life cycle thinking, industrial-urban symbiosis, product design for circularity, digitalization, sustainable transport, green jobs, health and safety, hazardous materials and waste, customer satisfaction, education and lifelong learning.

Associations of the chemical and process industries (Cefic, SusChem) and their projects (SPIRE, SIRA) have given a great added value; therefore, they should be practiced globally, at all the continents. The same globalization is suggested for the EGD. The companies and professional associations must respect the international agreements and conventions (SDGs, Paris agreement, EGD), declarations and recommendations.

There is no doubt that existing and innovative future technologies for efficient management of GHGs, water, energy and raw materials will play a decisive role in transforming current chemical and bio-chemical processes into more sustainable ones. Due to the high costs, some of these technologies would have to be co-financed by governments, while others could be implemented as long-term investments at the corporate level. For example, Norway has recently announced that it will finance a first large-scale carbon capture and storage project "Longship" [101] (1.5 billion €). The cement and the waste-to-energy plants involved in the project plan to reduce their CO<sub>2</sub> emissions by 50 % using capturing and storing CO<sub>2</sub> in a subsea reservoir in the North Sea. On the other hand, a Dutch brewery [102] has recently implemented an innovative green fuel alternative emerging in the form of metal powders [103]. Iron powder is considered as a high-density energy storage medium. It burns at high temperatures to form iron oxide, which can be reduced back to iron by electrolysis using renewable energy sources (e.g. photovoltaics) in a carbon-free cycle.

The decisive step towards more sustainable processes, regardless of available novel technologies, is the necessary change in mentality from chasing short-term financial gains to pursuing long-term sustainable financial, environmental, and social benefits. This step is required not only at the governance and corporate level, but also at the level of each individual.

Extrapolating from the past experiences, it is safe to say that advanced computational PSE tools will play an important role in the development of future chemical and biochemical processes. The process analysis, simulation and synthesis/optimization tools are now in general utilized in a sandbox mode – i.e. either in isolation from one another or in a sequential/iterative procedure. To identify truly innovative mitigating solutions and perhaps even restorative solutions, these tools would need to become inter-linked into a system that simultaneously enabled a detailed multi-scale modeling [104], process intensification (i.e. reduction in energy and resources demand, waste production and equipment size, out-of-the-box process solutions/schemes) [105] and LCSA Analysis.

Projects to develop sustainable processes are very demanding, both in terms of the knowledge and the financial investment required for their implementation. Projects in the field of circular economy often do not offer much added value. This is particularly problematic when it is cheaper to manufacture products from virgin sources than to process waste materials into secondary raw materials. The development and implementation of sustainable processes is highly interdisciplinary and includes laboratory research, tests at pilot plants, process setting up and commissioning. This is followed by the production and marketing of products and efficient waste management which includes the reuse, recycling, and processing of waste into added value products, fuels, secondary raw materials or energy recovery. There is no doubt that engineers are already developing efficient computer-aided tools for the development of sustainable technologies, including key enabling technologies, and sustainable processes, supply chains and networks that promote greater efficiency, waste reduction, closed loops and eco-design. But this will certainly not be enough to transform society from a linear to a circular economy. We believe that there is still a long way to go, as changes will be needed in many areas of society, i.e. at the level of business, education, finance, politics, legislation, and society as a whole.

At company level, efforts should focus on establishing and optimizing value chains in which stakeholders are linked to each other through raw material extraction, product manufacture, transport, collection, sorting and processing of waste into secondary raw materials, functional materials and energy. The aim should be to promote such industrial projects that balance economic efficiency, environmental impact, and social welfare. It is necessary to promote the growth of bio-based products and to seek market niches for such products.

In the field of education, young people must be encouraged to study science, technology, engineering, and mathematics (STEM), as these areas are crucial for the development of sustainable technologies and processes and for the circular economy. Curricula must be strengthened with attractive contents for young people and practical examples of green chemistry, cleaner production, eco-design, recycling, key enabling technologies, etc.

Experts in social sciences such as psychology and sociology must also be involved in the development of sustainable processes and products, as people need to change many deep-rooted habits and understand the impact of these changes on society and the environment in order to accept them as their own. The transition from a linear to a circular society must include the reduction of inequalities in society, more equity, justice, solidarity, participation, and involvement of citizens. Art must also be included, because products made from secondary raw materials, for example, must also be aesthetically designed if people are to accept them.

The development of sustainable technologies and the implementation of sustainable projects might require high financial investment, so the role of financial institutions and politics is also important. They must create the conditions for funding to be available for environmentally beneficial projects in the field of renewable energies, secondary raw materials, functional materials, key enabling technologies, etc. It is necessary to increase investment in education, research, innovations, and development.

The transition to the circular economy and the sustainable society can be promoted to a certain extent by political agreements and legal norms that impose restrictions on countries and companies with regard to emissions, proportions of recycled materials, the use of renewable resources and secondary raw materials, etc. In the long term, however, changes in existing political and broader social systems will be necessary in the direction of greater participation and balance, with the long-term sustainable progress of society and protection of the environment taking precedence over the partial interests of the individuals.

**Author Contributions:** Conceptualization, P.G.; methodology, P.G., Z.N.P. and M.B.; investigation, P.G., Z.N.P. and M.B.; writing—original draft preparation, P.G., Z.N.P. and M.B.; writing—review and editing, P.G., Z.N.P. and M.B.; supervision, P.G. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was co-funded by the Slovenian Research Agency (Research Program P2-0032 and Project J7-1816).

**Conflicts of Interest:** The authors declare no conflict of interest.

## References

1. Fisk, P. Megatrends 2020–2030 ... what they mean for you and your business, and how to seize the new opportunities for innovation and growth. Available online: <https://www.thegeniusworks.com/2019/12/mega-trends-with-mega-impacts-embracing-the-forces-of-change-to-seize-the-best-future-opportunities/> (accessed on 8 November 2020).
2. Ernst & Young. Are you reframing your future or is the future reframing you? EYQ 3<sup>rd</sup> Ed., 2020. Available online: [https://assets.ey.com/content/dam/ey-sites/ey-com/en\\_gl/topics/megatrends/ey-megatrends-2020-report.pdf](https://assets.ey.com/content/dam/ey-sites/ey-com/en_gl/topics/megatrends/ey-megatrends-2020-report.pdf) (accessed on 8 November 2020).
3. European Environment Agency, EEA, European environment – state and outlook 2015: Assessment of global megatrends. Available online: <file:///C:/Users/glavic/AppData/Local/Temp/Assessment%20of%20global%20megatrends-1.pdf> (accessed on 8 November 2020).
4. PricewaterhouseCoopers. PwC: 5 MegaTrends Affecting Your Business in 2019, Parts 1 and 2, 2017. Available online: <https://brandminds.live/pwc-5-megatrends-affecting-your-business-in-2019-2-of-2/> (accessed on 8 November 2020).
5. Moore, J.; Henbest, S. New Energy Outlook 2020, Executive Summary. BloombergNEF (New Energy Finance). Available online: [https://assets.bbhub.io/professional/sites/24/928908\\_NEO2020-Executive-Summary.pdf](https://assets.bbhub.io/professional/sites/24/928908_NEO2020-Executive-Summary.pdf) (accessed on 9 November 2020).
6. New Energy Outlook 2017, Bloomberg New Energy Finance. Available online: [https://data.bloomberglp.com/bnef/sites/14/2017/06/NEO-2017\\_CSIS\\_2017-06-20.pdf](https://data.bloomberglp.com/bnef/sites/14/2017/06/NEO-2017_CSIS_2017-06-20.pdf) (accessed on 9 November 2020).
7. European Commission, European Green Deal. Available online: [https://ec.europa.eu/clima/policies/eu-climate-action\\_en](https://ec.europa.eu/clima/policies/eu-climate-action_en) (accessed on 6 September 2020).
8. Ballweg, M.; Bukow, C.; Delasalle, F.; Dixon-Declève, S.; Kloss, B.; Lewren, I.; Metzner, J.; Okatz, J.; Petit, M.; Pollich, K.; Potočník, J.; Schwarzmanna, A.; Stuchtey, M.R.; Vincen, A. A System Change Compass – Implementing the European Green Deal in a Time of Recovery. 2020. Available online: <https://clubofrome.org/wp-content/uploads/2020/10/System-Change-Compass-Full-report-FINAL.pdf> (accessed on 7 November 2020).
9. TPE Design Engineering. Available online: <https://www.tpede.co.za/old-copies/process-design> (accessed on 15 October 2020).
10. Ellen MacArthur Foundation, Towards the Circular Economy, Vol. 1–2, 2013. Available online: <https://www.ellenmacarthurfoundation.org/assets/downloads/publications/Ellen-MacArthur-Foundation-Towards-the-Circular-Economy-vol.1.pdf> (accessed on 15 October 2020).
11. Montastruc, L.; Belletante, S.; Pagot, A.; Negny, S.; Raynal, L. From conceptual design to process design optimization: a review on flowsheet synthesis, Oil Gas Sci. Technol. – Rev. IFP Energies nouvelles 2019, 74, 80.
12. Computer Aided Process Engineering, Book series. Available online: <https://www.sciencedirect.com/bookseries/computer-aided-chemical-engineering/vol/46/suppl/C> (accessed on 15 October 2020).
13. European Commission, DG Environment, [https://ec.europa.eu/environment/sustainable-development/index\\_en.htm](https://ec.europa.eu/environment/sustainable-development/index_en.htm) (accessed on 15 October 2020).
14. World Business Council for Sustainable Development (WBCSD), Chemical Sector SDG Roadmap, 2018. Available online: [http://docs.wbcd.org/2018/07/Chemical\\_Sector\\_SDG\\_Roadmap.pdf](http://docs.wbcd.org/2018/07/Chemical_Sector_SDG_Roadmap.pdf) (accessed on 15 October 2020).
15. The European Chemical Industry Council (Cefic), A Solution Provider for Sustainability, 2019. Available online: <https://cefic.org/our-industry/a-solution-provider-for-sustainability/> (accessed on 15 October 2020).
16. European Center of Sustainable Development (ECSDev). Available online: <https://ecsdev.org/> (accessed on 16 October 2020).



17. Conference on Engineering Sustainable Development 2019 co-hosted by AIChE-APRU. Available online: <https://apru.org/event/2019-international-conference-on-technical-and-engineering-challenges-of-addressing-sustainable-development/> (accessed on 16 October 2020).
18. Anastas, P. T.; Zimmerman, J. B. Design through the Twelve Principles of Green Engineering, *Env. Sci. Tech.* **2003**, 37(5), 94A–101A.
19. Anastas, P. T.; Warner, J. *Green Chemistry, Theory and Practice*, Oxford University Press, London, 1998.
20. Gagnon, B.; Leduc, R.; Savard, L. Sustainable development in engineering: a review of principles and definition of a conceptual framework, *Env. Eng. Sci.* **2009**, 26(10), 1459–1472.
21. The Royal Society of Engineering, *Engineering for Sustainable Development: Guiding principles*, London, 2005.
22. American Chemical Society, Green Chemistry Institute, *Design Principles for Sustainable and Green Chemistry and Engineering*, Washington. Available online: <https://www.acs.org/content/acs/en/greenchemistry/principles.html> (accessed on 16 October 2020).
23. Crul, M. R. M., Diehl, J. C. (2006). *Design for sustainability: a Step by Step Approach*. 2009, UNEP, Paris. Available online: <https://wedocs.unep.org/handle/20.500.11822/8742> (accessed on 16 October 2020).
24. Ceschin, F. Evolution of design for sustainability: From product design to design for system innovations and transitions, *Design Studies* **2016**, 47, 118–163.
25. Acaroglu, L. Quick Guide to Sustainable Design Strategies. Available online: <https://medium.com/disruptive-design/quick-guide-to-sustainable-design-strategies-641765a86fb8> (accessed on 17 October 2020).
26. Biegler, L. T.; Grossman, I. E.; Westerberg, A. W. *Systematic Methods of Chemical Process Design*, Prentice Hall, New Jersey, 1999.
27. Koolen, J. L. A. *Design of Simple and Robust Process Plants*, Wiley-VCH, Weinheim, 2001.
28. Smith, R., *Chemical Process: Design and Integration*, 2<sup>nd</sup> Ed., Wiley, 2014.
29. Bernecker, G. *Planung und Bau verfahrenstechnischer Anlagen*, Springer, Berlin, 2001.
30. Allen, D.; Shonnard, D. R. *Sustainable Engineering: Concepts, Design and Case Studies*, Pearson, 2012.
31. Perl, J., *Sustainability Engineering: A Design Guide for the Chemical Process Industry*, Springer, eBook. Available online: <https://www.springer.com/gp/book/9783319324937> (accessed 9 November 2020).
32. Luu, L. Q.; Halog, A. Life Cycle Sustainability Assessment; A Holistic Evaluation of Social, Economic, and Environmental Impacts, in *Sustainability in the Design, Synthesis and Analysis of Chemical Engineering Processes* Eds Ruiz-Mercado, G., Cabezas, H.), Elsevier Science Direct, 2016.
33. Scopus, Document search. Available online: <https://www.scopus.com/search/form.uri?display=basic> (31 October 2020).
34. Web of Science, Core Collection Results. Available online: [http://apps.webofknowledge.com/Search.do?product=WOS&SID=F4AauXxtQuY92K5WeIQ&search\\_mode=GeneralSearch&prID=9b5b11c6-5dfb-4e80-b5eb-3143c6c4f66b](http://apps.webofknowledge.com/Search.do?product=WOS&SID=F4AauXxtQuY92K5WeIQ&search_mode=GeneralSearch&prID=9b5b11c6-5dfb-4e80-b5eb-3143c6c4f66b) (accessed on 30 September 2020).
35. Nikolopoulou, A.; Ierapetritou, M. A. Optimal design of sustainable chemical processes and supply chains: A review. *Comput. Chem. Eng.* **2012**, 44, 94–103.
36. Kumar, A.; Sah, B.; Singh, A. R.; Deng, Y.; He, X.; Kumar, P.; Bansal, R. C. A review of multi criteria decision making towards sustainable renewable energy development. *Renew. Sust. Energ. Reviews* **2017**, 69, 596–609.
37. Corominas, L.; Foley, J.; Guest, J. S.; Hospido, A.; Larsen, H. F.; Morera, S.; Shaw, A. Life cycle assessment applied to wastewater treatment: State of the art. *Water Res.* **2013**, 47(15).
38. Li, S.; Mirlekar, G.; Ruiz-Mercado, G. J.; Lima, F. V. Development of Chemical Process Design and Control for Sustainability. *Processes* **2016**, 4(3), 23.
39. Bare, J. TRACI 2.0: The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts 2.0. *Clean Technol. Envir.* **2011**, 13(5), 687–696.
40. Klewitz, J.; Hansen, E. G. Sustainability-Oriented Innovation of SMEs: A Systematic Review. *J. Clean. Prod.* **2014**, 65, 57–75.

41. Siddique, Md. N. I.; Wahid, Z. Ab. Achievements and perspectives of anaerobic co-digestion: A review. *J. Clean. Prod.* **2018**, *194*, 359–371.
42. Singh S. V.; Ming, Z.; Fennell P. S.; Shah, N.; Anthony, E. J. Progress in biofuel production from gasification. *Prog. Ener. Combust.* **2017**, *61*, 189–248.
43. Babazadeh, R.; Razmi, J.; Pishvae, M. S.; Rabbani, M. A sustainable second-generation biodiesel supply chain network design problem under risk. *Omega* **2017**, *66*(B), 258–277.
44. Mata, T. M.; Martins, A. A.; Caetano, N. S. Microalgae for biodiesel production and other applications: A review. *Renew. and Sust. Energ. Rev.* **2010**, *14*(1), 217–232.
45. Santibañez-Aguilar, J. E.; González-Campos, J. B.; Ponce-Ortega, J. M.; Serna-González, M.; El-Halwagi, M. M. Optimal Planning of a Biomass Conversion System Considering Economic and Environmental Aspects. *Ind. Eng. Chem. Res.* **2011**, *50*(14), 8558–8570.
46. Murray, A.; Skene, K.; Haynes, K.. The Circular Economy: An Interdisciplinary Exploration of the Concept and Application in a Global Context. *J. Bus. Ethics* **2017**, *140*, 369–380.
47. Walmsley, T. G.; Ong, B. H. Y.; Klemenš, J. J.; Tan, R. R.; Varbanov, P. S. Circular Integration of processes, industries, and economies. *Renew. and Sust. Energ. Rev.* **2019**, *107*(C), 507–515.
48. Knez, Ž.; Markočič, E.; Leitgeb, M.; Primožič, M.; Knez Hrnič, M.; Škerget, M. Industrial applications of supercritical fluids: A review. *Energy* **2014**, *77*, 235–243.
49. Roy, R. Sustainable product-service systems, *Futures* **2000**, *32*(3–4), 289–299.
50. Galli, B.J. How to Effectively Use Economic Decision-Making Tools in Project Environments and Project Life Cycle. *IEEE T. Eng. Manage.* **2020**, *67*(3), 932–940.
51. Khalid, M.; Aguilera, R.P.; Savkin A.V.; Agelidis, V.G. On maximizing profit of wind-battery supported power station based on wind power and energy price forecasting. *Appl. Energ.* **2018**, *211*, 764–773.
52. Nicoletti, J.; Ning, C.; You, F. Optimizing return on investment in biomass conversion networks under uncertainty using data-driven adaptive robust optimization. Proceedings of the 29th European Symposium on Computer Aided Process Engineering, Eindhoven, The Netherlands, June 16th to 19th, 2019; Kiss, A.A., Zondervan, E., Lakerveld, R., Özkan, L., Eds.; Elsevier: Amsterdam, Netherland, 2019; 67–72.
53. Ziyai, M.R.; Mehrpooya, M.; Aghbashlo, M.; Omid, M.; Alsagri, A.S.; Tabatabaei, M. Techno-economic comparison of three biodiesel production scenarios enhanced by glycerol supercritical water reforming process. *Int. J. Hydrogen Energ.* **2019**, *44*, 17845–17862.
54. Novak Pintarič, Z.; Kravanja, Z. Selection of the economic objective function for the optimization of process flow sheets. *Ind. Eng. Chem. Res.* **2006**, *45*, 4222–4232.
55. Cisternas, L.A.; Lucay F.; Gálvez E.D. Effect of the objective function in the design of concentration plants. *Miner. Eng.* **2014**, *63*, 16–24.
56. Kasaš, M.; Kravanja, Z.; Novak Pintarič, Z. Suitable modeling for process flow sheet optimization using the correct economic criterion. *Ind. Eng. Chem. Res.* **2011**, *50*, 3356–3370.
57. Kasaš, M.; Kravanja, Z.; Novak Pintarič, Z. Achieving Profitably, Operationally, and Environmentally Compromise Flow-Sheet Designs by a Single-Criterion Optimization. *AIChE J.* **2012**, *58*, 2131–2141.
58. Argoti, A.; Orjuela, A.; Narváez, P.C. Challenges and opportunities in assessing sustainability during chemical process design. *Curr. Opin. Chem. Eng.* **2019**, *26*, 96–103.
59. Lee, Y.S.; Graham, E.J.; Galindo, A.; Jackson, G.; Adjiman, C.S. A comparative study of multi-objective optimization methodologies for molecular and process design. *Comput. Chem. Eng.* **2020**, *136*, 106802.
60. Wang, Z.; Parhi, S.S.; Rangiah, G.P.; Jana, A.K. Analysis of Weighting and Selection Methods for Pareto-Optimal Solutions of Multiobjective Optimization in Chemical Engineering Applications. *Ind. Eng. Chem. Res.* **2020**, *59*, 14850–14867.
61. TU Delft. Data on eco-costs 2017, Available online: [www.ecocostsvalue.com/EVR/model/theory/subject/5-data.html](http://www.ecocostsvalue.com/EVR/model/theory/subject/5-data.html) (accessed on 26 10 2020).
62. Novak Pintarič, Z.; Varbanov, P.S.; Klemenš, J.J.; Kravanja, Z. Multi-Objective Multi-Period Synthesis of Energy Efficient Processes under Variable Environmental Taxes. *Energy* **2019**, *189*, 116182.
63. Bubicz, M.E.; Barbosa-Póvoa, A.P.F.D.; Carvalho, A. Incorporating social aspects in sustainable supply chains: Trends and future directions. *J. Clean. Prod.* **2019**, *237*, 117500.
64. Zore, Ž.; Čuček, L.; Kravanja, Z. Synthesis of sustainable production systems using an upgraded concept of sustainability profit and circularity. *J. Clean. Prod.* **2018a**, *201*, 1138–1154.

65. Zore, Ž.; Čuček, L.; Širovnik, D.; Novak Pintarič, Z.; Kravanja, Z. Maximizing the sustainability net present value of renewable energy supply networks. *Chem. Eng. Res. Des.* **2018b**, *131*, 245-265.
66. Fan, Y.V.; Chin, H.H.; Klemeš, J.J.; Varbanov, P.S.; Liu, X. Optimisation and process design tools for cleaner production. *J. Clean. Prod.* **2020**, *247*, 119181.
67. López-Delgado, A.; Robla, J.I.; Padilla, I.; López-Andrés, S.; Romero M. Zero-waste process for the transformation of a hazardous aluminum waste into a raw material to obtain zeolites. *J. Clean. Prod.* **2020**, *255*, 120178.
68. Salkuyeh, Y.K.; Adams II, T.A. Integrated petroleum coke and natural gas polygeneration process with zero carbon emissions. *Energy* **2015**, *91*, 479-490.
69. Karka, P.; Papadokonstantakis, S.; Kokossis, A. Environmental impact assessment of biomass process chains at early design stages using decision trees. *Int. J. Life Cycle Ass.* **2019**, *24*, 1675-1700.
70. Mangili, P.V.; Prata, D.M. Preliminary design of sustainable industrial process alternatives based on eco-efficiency approaches: The maleic anhydride case study. *Chem. Eng. Sci.* **2020**, *212*, 115313.
71. Geissdoerfer, M.; Savaget, P.; Bocken, N.M.P.; Hultink, E. J. The Circular Economy - A new sustainability paradigm?. *J. Clean. Prod.* **2017**, *143*, 757-768.
72. Yáñez, M.; Ortiz, A.; Brunaud, B.; Grossmann, I.E.; Ortiz, I. The use of optimization tools for the Hydrogen Circular Economy. Proceedings of the 29th European Symposium on Computer Aided Process Engineering, Eindhoven, The Netherlands, June 16th to 19th, 2019; Kiss, A.A., Zondervan, E., Lakerveld, R., Özkan, L., Eds.; Elsevier: Amsterdam, Netherland, 2019; 1777-1782.
73. Klemeš, J.J.; Fan, Y.V.; Jiang, P. Plastics: friends or foes? The circularity and plastic waste footprint. *Energ. Source. Part A* **2020**, Available online: <https://doi.org/10.1080/15567036.2020.1801906>.
74. Avraamidou, S.; Baratsas, S.G.; Tian, Y.; Pistikopoulos, E.N. Circular Economy - A challenge and an opportunity for Process Systems Engineering. *Comput. Chem. Eng.* **2020**, *133*, 106629.
75. Genc, A.; Zeydan, O.; Sarac, S. Cost analysis of plastic solid waste recycling in an urban district in Turkey. *Waste Manage. Res.* **2019**, *37*(9), 906-913.
76. Umeda, T.; Itoh, J.; Shikoro, K. Heat Exchanger Synthesis. *Chem. Eng. Prog.* **1978**, *74*, 70-76.
77. Linnhoff, B.; Hindmarsh, E. The pinch design method for heat exchanger networks. *Chem. Eng. Sci.* **1983**, *38*(5), 745-763.
78. Austin, N.D.; Sahinidis, N.V.; Trahan, D.W. Computer-aided molecular design: An introduction and review of tools, applications, and solution techniques. *Chem. Eng. Res. Des.* **2016**, *116*, 2-26.
79. Strniša, F.; Tatiparthi V.S.; Djinoić, P.; Pintar, A.; Plazl, I. Ni-containing CeO<sub>2</sub> rods for dry reforming of methane: Activity tests and a multiscale lattice Boltzmann model analysis in two model geometries. *Chem. Eng. J.* **2020**, Available online: <https://doi.org/10.1016/j.cej.2020.127498> (accessed on 1 November 2020).
80. Rossetti, I. Reactor Design, Modelling and Process Intensification for Ammonia Synthesis. In *Sustainable Ammonia Production*; Inamuddin; Boddula R.; Asiri A.M., Eds.; Green Energy and Technology, Springer, 2020, pp 17-48.
81. Dimian, A.C.; Bildea, C.S.; Kiss, A.A. Methanol. In *Applications in Design and Simulation of Sustainable Chemical Processes*; Dimian, A.C.; Bildea, C.S.; Kiss, A.A., Eds.; Elsevier, 2019; pp 101-145.
82. Tula, A.K.; Eden, M.R.; Gani, R. Process synthesis, design and analysis using a process-group contribution method. *Comput. Chem. Eng.* **2015**, *81*, 245-259.
83. Zhang, X.; Song, Z.; Zhou, T. Rigorous design of reaction-separation processes using disjunctive programming models. *Comput. Chem. Eng.* **2018**, *111*, 16-26.
84. Potrč, S.; Čuček, L.; Zore, Ž.; Kravanja, Z. Synthesis of Large-Scale Supply Networks for Complete Long-term Transition from Fossil to Renewable-based Production of Energy and Bioproducts. *Chem. Eng. Trans.* **2020**, *81*, 1039-1044.
85. Xu, D.; Lv, L.; Ren, J.; Shen, W.; Wei, S.; Dong, L. Life Cycle Sustainability Assessment of Chemical Processes: A Vector-Based Three-Dimensional Algorithm Coupled with AHP. *Ind. Eng. Chem. Res.* **2017**, *56*(39), 11216-11227.
86. Zore, Ž.; Čuček, L.; Kravanja, Z. Syntheses of sustainable supply networks with a new composite criterion – Sustainability profit. *Comput. Chem. Eng.* **2017**, *102*, 139-155.
87. ANSYS. Ansys: Engineering Simulation & 3D Design Software. Available online: [www.ansys.com](http://www.ansys.com) (accessed on 15 October 2020).
88. OpenFOAM. The open source CFD toolbox. Available online: [www.openfoam.com](http://www.openfoam.com) (accessed on 15 October 2020).

89. AspenPlus. The Leading Process Simulation Software in the Chemical Industry. Available online: [www.aspentech.com](http://www.aspentech.com) (accessed on 15 October 2020).
90. DWSIM. DWSIM-Chemical Process Simulator Available online: [dwsim.inforside.com.br](http://dwsim.inforside.com.br) (accessed on 15 October, 2020).
91. GAMS. The general algebraic modelling system. Available online: [www.gams.com](http://www.gams.com) (accessed on 15 October 2020).
92. PYOMO. Available online: [www.pyomo.org](http://www.pyomo.org) (accessed on 15 October 2020).
93. GABY. Gaby-Software. Available online: [www.gabi-software.com](http://www.gabi-software.com) (accessed on 15 October 2020).
94. OpenLCA. The Life Cycle and Sustainability Software. Available online: [www.openlca.org](http://www.openlca.org) (accessed on 15 October 2020).
95. IDEAS PSE Framework. Available online: <https://idaes.org/>, (accessed on 15 October 2020).
96. MIPSYN-GLOBAL. Available online: <http://mipsyn-global.fkkt.um.si/> (accessed online 15 October 2020).
97. Cefic, Facts and Figures, 2020. Available online: <https://cefic.org/app/uploads/2019/01/The-European-Chemical-Industry-Facts-And-Figures-2020.pdf> (accessed on 4 October 2020).
98. Cefic sustainability Charter. Available online: <https://cefic.org/app/uploads/2019/01/Cefic-Sustainability-Charter-TeamingUp-For-A-SustainableEurope.pdf> (accessed on 4 November 2020).
99. SusChem, European Technology Platform for Sustainable Chemistry. Strategic Innovation and Research Agenda, SIRA. Available online: <https://cefic.org/app/uploads/2020/02/SusChem-SIRA-2020.pdf> (accessed on 6 September 2020).
100. Sustainable Process Industry through Resource and Energy Efficiency, SPIRE 2050 Vision, 2018. Available online: <https://cefic.org/app/uploads/2019/02/SPIRE-vision-2050.pdf> (accessed on 6 November 2020).
101. Hjuske, A.K. The Government launches 'Longship' for carbon capture and storage in Norway. Available online: <https://bit.ly/3ewvVUI> (accessed on 18 October 2020).
102. Blain, L. World first: Dutch brewery burns iron as a clean, recyclable fuel. Available online: <https://bit.ly/2JEZeJb> (accessed on 5 November 2020).
103. Bergthorson, J.M. Recyclable metal fuels for clean and compact zero-carbon power. *Prog. Energ. Combust.* **2018**, *68*, 169–196.
104. Floudas, C.A.; Niziolek, A.M.; Onel, O.; Matthews, L.R. Multi-scale systems engineering for energy and the environment: Challenges and opportunities. *AIChE J.* **2016**, *62*(3), 602–623.
105. Bielenberg, J.; Palou-Rivera, I. The RAPID Manufacturing Institute – Reenergizing US efforts in process intensification and modular chemical processing. *Chem. Eng. Process.* **2019**, *138*, 49–54.