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Trends in sustainable process design - from molecular to global scales

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Highlights

- Sustainability issues are changing the nature of process design problems and methods.
- Design boundaries have expanded down towards molecular level and up to global scales.
- Methods and decision support frameworks address multidimensionality and multiscale.
- Explicit consideration of ecosystems has shown recent advancements.
- Tools capturing the full range of scales and interactions are yet to be developed.

Abstract

The quest for sustainability is changing how chemical engineers conceptualise new processes. The task also becomes more complicated by economic and social uncertainties, local diversity of renewable resources and globalisation. These realities are changing the nature of process design problems and recent advancements have been able to incorporate the multidimensionality and multiscale boundaries by exploiting the power of mathematical methods, decision support frameworks and insight based methods. In doing so, two main trends for methods development can be distinguished, the ones considering expanded boundaries for design from the lowest molecular level to the process level, and the ones from process to the higher levels of value chains, ecosystems and the planet. However, a truly integrated framework that captures the full range of scales and interactions from molecular to planetary levels is yet to be developed to be able to find superior designs that perhaps we had never thought of before.

Keywords: chemical process, sustainability, optimisation, design methods

Introduction

Extensive consumption of coal, oil, gas and synthetic fertilisers have led to excessive greenhouse gas (GHG) accumulation in the atmosphere. The resulting increased capacity to absorb solar irradiation produces the energy imbalance that drives climate change. Under this context, the capacity of the planet to provide food, energy and clean water become more constrained [1]. Longer dry seasons in some localities means less water available and less agricultural production, while more energy is consumed for thermal comfort. These issues revealed the tight coupling between human and natural components into a complex nexus that needs to be understood using systems integration approaches for truly sustainable solutions [2]. Chemical engineering with its inherent systems view is arguably the discipline best positioned to address these issues. The chemical industry transforms raw materials into goods, electricity and heat that enable modern lifestyles. In doing so, 7 % of global industrial greenhouse gas (GHG) emissions are generated [3]. The chemical industry also helps to save energy and emissions by supplying innovative insulation and lightweight materials, fuel additives, catalysts, and enzymes as well as biotechnological products such as biofuels and chemical alternatives to petrochemicals. However, there is still wider scope for improving and designing processes with sustainability in mind. In fact, this has propelled the development of systematic tools and methods to unravel interactions that are critical for achieving sustainable process designs.

The quest for sustainability is changing how chemical engineers conceptualise new processes, as consideration should be given not only to reactions, separations, energy efficiency, and economics but also to safety, environmental and social impacts. Until the last century, chemical processes were traditionally designed with the plant gates as boundaries and with economics as the primary objective, often neglecting consequences for the environment. Awareness of detrimental environmental impacts by human activities encouraged governments to put regulations in place, and the industry then adopted end-of-pipe solutions to treat wastes and emissions. With the oil crisis of the 1970s, energy efficiency became essential and gave light to the pinch analysis method for process integration, which has helped to save up to 30% of energy use in process industries while reducing related emissions [4]. The importance of preserving vital resources such as water and reducing carbon emissions have also driven the development of similar methods. Arguably, process integration has been the major research contribution from what it is known as process systems engineering (PSE), towards making chemical processes more sustainable. Nowadays, there are two main approaches for process design, hierarchical methods using heuristics and insight-based approaches (e.g. pinch analysis methods) [5] and mathematical optimisation methods [6]••. In the recent literature there is much more effort put into developing the second type of methods, with recent advances in multiobjective optimisation and optimisation under uncertainty for robust process designs [7]. These approaches are much needed to address the multifaceted concept of sustainability. However, hybrid methods are preferable to make a balance between insights and complex mathematical formulations for a better appreciation of the decision-making process and the solutions obtained.

Figure 1 shows an onion model with the various levels or boundaries that are now considered in recent developments for sustainable process design. This review focuses on how the need to look at multiple scales or levels of process systems is expanding the boundaries considered for design; and how such an expansion is influencing current developments and applications of methods for sustainable process design. This has been clearly reflected in the trends in the literature reviewed from 2015 to date. The first section reviews recent works looking down towards the molecular level. The second section reviews recent works that consider expanded system boundaries from process level up to value chain and wider systems. A prospective section then provides a synthesis of challenges and opportunities for developing sustainable process designs.

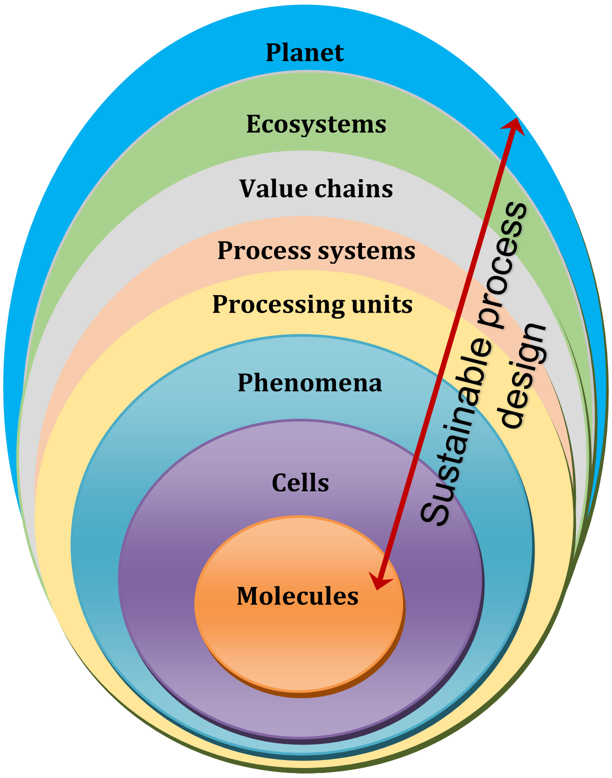

Figure 1 Levels considered in recent trends for sustainable process design

From molecules to process flowsheets

By looking at the molecular level, researchers understand molecular interactions to target more efficient solvents, reactants and catalysts. This contributes towards making processes more sustainable by reducing the use of toxic solvents, energy consumption and waste generation. Advances in computational power and group contribution methods for predicting physicochemical properties have propelled the area of computer-aided molecular and process design (CAMPD), which views the molecular level as an entry point for sustainable process design [8] [9]. A method has been recently developed by introducing a new kind of solvent descriptor obtained from quantum chemical calculations [10]. The method simultaneously optimises solvent molecular structures and processing units using a mixed-integer nonlinear program for a Diels–Alder reaction. A rather hierarchical method has been applied to the design of an absorption process to separate carbon dioxide from methane [11]. This process can potentially contribute to making high purity methane, from shale gas and biogas, ready for injection into current infrastructure. The methods reviewed can be so computationally expensive that their application may not be practical. However, efficient algorithms for the application of group contribution methods are being developed [12]. Methods based on quantum calculations have been able to find best solvent candidates that minimise energy requirements by up to 63% [13] •.

Molecular level methods are primarily applied to solvent-based separations. Consideration of the full process system can create scopes for better process integration and intensification, which potentially lead to innovative designs. This is a challenge yet to be addressed mainly because of the complexity of mathematical formulations for CAMPD problems. However, CAMPD inspired new methods by making analogies between functional groups in a molecule and the distinctive functionality of a processing unit or group of units. Automated flowsheet generation based on the concept of functional process-groups and connectivity rules is able to generate structurally feasible flowsheet alternatives [14]••. The framework allows fast screening of alternatives due to the "property" models for energy consumption, atom efficiency and environmental impacts of individual process-groups. This provides an advancement towards incorporating sustainability from early stages in the process design. The analogy to molecular group contribution methods has been taken further to develop a process synthesis and intensification methodology using phenomena (e.g. reaction, convection, diffusion, etc.) as building blocks of processing units and flowsheets [15] ••. Although the last two methods rely on some mathematical algorithms, they still require knowledge inputs from the engineer to pre-define combinatorial rules and constraints for feasible flowsheets, which may favour their wider adoption if they can be implemented into a user-friendly software [16]. Despite the innovative outcomes, validation of unit operations and flowsheets would still be needed.

Other interesting developments that are expanding the boundaries for process design are synthetic biology and metabolic engineering [17]. Multiscale modelling methods that are able to model relatively large physical systems and capture the essential features of the micro- and nanoscale structure and interactions inside the cells are urgently needed for developing sustainable bioprocesses [18]. This will benefit from recent novel approaches that integrate experimental studies with process synthesis and simulation [19], [20]. Promising research directions for developing renewable fuel production processes have been identified by using this "process-first" approach [21] •.

From process to global systems

Recent advances at the process level show that it is possible to automate process design, heat integration and utility system design using superstructure optimisation [22]. Process integration approaches keep developing for higher system levels including techniques for carbon and other environmental footprint problems [23] •. However, it is becoming more and more important to recognise that chemical process systems are part of a system of systems. This has pushed forward research into new approaches that address the necessary expansion of boundaries for design towards the large scales, including eco-industrial parks, value chains, techno-ecological systems and global planet systems.

Eco-industrial parks (EIP) have been undertaken as an object of study by PSE from planning and design points of view, mainly using mathematical optimisation [24][25] [26]•. This expanded the boundaries to co-located processing plants and often involve multiple stakeholders that can influence design decisions. Fuzzy optimisation methods have been applied to bioenergy parks [27], while game theory has been used for designing water networks [28]. A hybrid approach integrating hierarchical decision making and multiobjective optimisation has proved useful [29]. The advantage of these methods is the integration of the multiple stakeholder preferences, roles and importance; because of this, their application can provide attainable solutions. Waste reuse and by-product synergies in EIP can also be optimised using mathematical approaches [30]. Material flow analysis [31] and input-output analysis [32]•• are other techniques from the area of industrial ecology that have been used for designing EIP. Sustainability indicators have also been developed to assess the performance of EIP [33].

At the supply chain level, robust multiobjective optimisation methods have been developed to address the geographical and temporal diversity of renewable resources, wider system boundaries and uncertainties [34]. The identification of relevant trade-offs is also necessary to gain insights of the solution space [35]. Recent advancements also demonstrate the benefits of incorporating spatially and temporally explicit models for the design of synthetic natural gas supply chains [36], biomass value chains with multifeedstock and multivector energy systems [37] and hydrogen networks with transport and storage [38]. Designing renewable energy supply chains has also been performed using the P-graph method considering variable inputs and outputs and processes with multiperiod operations [39][40][41] ••. Biofuel and biorefinery value chains create further challenges and opportunities such as diversity of biomass feedstock and conversion technologies [42] [43]. A more general review identifies the multiscale, multiobjective and multiplayer natures of the value chain design problem as the major challenges [44] ••. Some of these challenges have been addressed for multiplayer shale gas supply chains using net present value and GHG emissions as optimisation objectives [45].

A supply chain model incorporating land use and ecosystem services is a notable contribution that demonstrates how the boundaries for design are increasingly expanding [46]. Conceptualising processes in synchrony and synergy with the ecological processes has also shown significant advances, including a novel framework to develop techno-ecological synergy as a strategy for sustainable process design [47]•. It is also important to ensure technologies are implemented according to the capacity of local ecosystems [48] [49]. The local scale can also facilitate more opportunities for direct synergetic interactions, which can be facilitated by a framework that explicitly captures the dynamic nature of ecosystems as well as techno-ecological interactions in locally integrated production systems [50]. The design of local systems should also recognise the global planetary system as the ultimate boundary for process design by employing a process-to-planet framework [51]••.

A more recent trend is the consideration of the food-energy-water nexus concept as an approach to integrated resource management and secure access to basic human needs. Indeed PSE has a great opportunity for application of methods to create positive synergies among the nexus subsystems [52]••. Studies on simultaneous optimisation start to appear, such as water and energy optimisation [53], and more recently the local integration of food, energy and water subsystems [54]. Other systems concepts influencing recent developments include polygeneration, which encloses many of current ideas for multifeedstock, multiproduct and multifunctional process systems [55], [56]. The circular economy or closed loop concept is also influencing the trends in process design, including novel concepts for waste processing and resource recovery [57] [58] [59]. Another trend is the design of energy self-sufficient processes involving hybrid production systems combining renewable energy sources and fuel and chemical production [60][61][62] [63]. There is also a trend on co-processing of biomass and fossil feedstocks as a bridge between current fossil based economy and a future bio-economy [64].

The developing of multicriteria decision (MCD) support frameworks and indicators for application during early design stages is another trend that addresses the need for a transparent decision-making process and to facilitate engagement of decision makers [65][66] [67]. A new multilevel framework proposes a joint risk assessment matrix for the assessment of process alternatives [68]. Similar frameworks have been developed for biomass processing paths and biorefinery processes [69] [70] [71]. Methods based on indicators adopted from green chemistry and engineering have also been developed to assist decision making during process design [72][73][74]••. Frameworks considering triple bottom line sustainability criteria are desirable to have a comprehensive and tractable overview of process design performances In this respect, the novel Decision-Support Framework Integrating Economic, Environmental and Social Sustainability (DESIRES) is a unique contribution [75]••.

Prospective for sustainable chemical process design

Process design should optimise resources as well as minimise impacts by means of resource recovery and extensive feedstock fractionation, which enables a wider scope for process integration and intensification. Designs should also enable synergistic linkages with other production components in the form of industrial parks as well as with the ecosystems in the form of techno-ecological systems. In this way circularity of resources for their preservation for the future generations can be enabled, thus achieving the ultimate goal of sustainability. With the rise of widely distributed biomass and other renewable resources, it is also necessary to capture their spatial and temporal diversity as well as their role in the global economy. Therefore, new methods and tools need to be able to capture such new requirements and realities which drive the boundary expansion for process design, at the lowest scale towards molecules and cells; at the larger scales towards value chains, techno-ecological systems and the planet.

Despite significant advancements at both sides of the scales, a truly integrated framework that captures the full range of scales and interactions from molecular to planetary levels is yet to be developed to be able to find innovative designs that perhaps we had never thought of before. Design and analysis methods, solution algorithms and visualisation of multiple indicators for such integrated framework will be necessary. Across the various scales, only a few methods include social indicators. Furthermore, systematic methodologies for reducing the multidimensionality of indicators by maintaining the most relevant ones are also lacking.

Although sophisticated mathematical methods have proved useful in theory, results need to be validated experimentally and operationalised by user-friendly software tools for application in the engineering practice. This requires the computationally efficient coupling of heterogeneous models of multiple temporal and spatial scales that should be flexible enough for wide applications. The tool should allow solutions to remain trackable to the decision maker so that the path followed by the solver can be examined to gain knowledge that can be applied in other contexts without solving complex optimisation problems. There is the possibility to benefit from recent advancements in data analytics and machine learning algorithms which promise to take PSE and process design methods to new avenues.

Adapting to growing knowledge and understanding at the molecular level and catching up with advancements in systems biology and metabolic engineering is another challenge. This also makes clear that a multidisciplinary approach including chemistry, biology, ecology, economy and social sciences is also necessary. Thus, the future of process design also lies on a collaborative approach to finding sustainable solutions since early stages of development.

Finally, the widespread application of the recent advances also requires the development of educational materials to equip future generations of chemical engineers with the required tools and systems thinking for developing sustainable process [76] [77][78]••.

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