Challenges and future directions for process and product synthesis and design

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ABSTRACT

The incorporation of renewable energy sources to the market has brought a new golden era for process synthesis with challenges and opportunities. In this work, we give a brief review of the state of the art and then present challenges and future directions in this exciting area. The biggest driver is the rapid improvement in computer technology which greatly increases the number of factors that can be considered during the design process. Thus, some of the key future directions lie in integrating the design process with other aspects of process systems engineering, such as scheduling, planning, control, and supply chain management. In addition, sustainability is now a major consideration. The tools available to address these challenges are limited but we are in a position to develop them based on strong chemical engineering principles following a multidisciplinary approach with contributions from other disciplines including biology, biochemistry, computer science, materials, and chemistry.

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1. Introduction

The first contribution in the field of process synthesis is widely acknowledged to date back to 1973 (Rudd et al., 1973) where the theoretical background was established. Traditionally, the field represents the methodological creation of a process to produce chemical products using experience, heuristics, and algorithms. Over time, the boundaries of the analysis expanded as more and more complex concepts and techniques are developed, allowing for more layers of rigor to be considered. This included fields such as optimization, modelling, economics, and control, which ultimately resulted in better process designs. However, product design was traditionally considered to be more related to consumer marketing than chemical engineering. Only recently has product design become a part of the scope of process engineers, driven in part by early contributions of Ng et al. (2007) and many others including a textbook (Cussler and Moggridge, 2011). For example, the popular textbook Product and Process Design Principles (Seider et al., 2017) did not get the "Product and" part of the title until the second edition. However, it is only natural that the boundaries of process design have now expanded to include product design since the next level up from the question "What is the best process to make this product?" is "What product should we make to meet

market needs?" These products can range from custom chemicals such as catalysts for reactors, solvents for CO_2 capture, or thermal fluids for Rankine cycles to complex products such as cosmetics, pharmaceuticals, and processed food.

Therefore, both fields must be considered within an integrated approach in order to be able to handle the tradeoffs between them. For instance, to manufacture a particular chemical product we need a process that meets certain constraints such as pressure, temperature, or materials of construction. Alternatively, we may want to develop flexible processes for the production of a range of different products, such as consumer products, which is limited by process constraints. Since the product ultimately depends on the process, this creates a strong link between them as parts of the larger supply chain. For example, chemical processes must be controlled and operated carefully as they are the core of the product supply chain. And, since more recent trends in chemical processing indicate a new focus on using renewable resources such as biomass, solar, or wind energy into the supply chain this fact adds additional challenges with regards to consistency and irregular availability of these resources. Furthermore, because all of these are linked together through the supply chain, this implies that improvements to upstream sections of the chain can yield economic benefits in the final products far downstream. For example, improved logistics and operations in handling the complex spatial and temporal challenges issues associated with renewable energy harvesting far upstream can greatly improve product quality (or

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economics) of the products. Thus, as this paper will show, the general trend in process and product design has been to move away from separate silos of thought and instead be considered together, as we become better able to handle more complex tasks. And, as we will show, the next frontier is to expand the scope farther, such as the consideration of larger aspects of the supply chain, the integration of process control, and other issues.

This work is divided in five sections plus conclusions. First, a brief overview of the traditional focus of this area is presented from the heuristic and mathematical optimization perspectives. Note that the aim is not to provide a thorough review; other papers in the literature are more detailed for process design (Westerberg, 2004; Barnicki and Siirola, 2004), but they do not cover product design nor the integration between process and product design. Furthermore, our aim is to provide background that will help understand the challenges that new processes and resources pose on the chemical and energy industries. Section 3 focuses on major challenges within the field of process and product design that are being addressed through current research. Subsequently, Section 4 presents some potential research future directions which currently do not receive a large amount of research attention but are likely to be the next major areas of research interests. Finally Section 5 introduces the PSE tree wiki as a way to help the design community link concepts, information and references within the process and product area in order to help researchers better address increasingly complex design problems.

2. A bit of history

In this section we highlight the research trends over the last 40–50 years on process and product design presenting the problems addressed, showing different methodologies to deal with the same problem as well as the development of methods and tools to address more realistic problems over time. Detailed reviews focusing on process design have been published over the years (Westerberg, 2004; Barnicki and Siirola, 2004). An important issue to highlight is the fact that for years process design was addressed separately from product design and only lately both fields have converged to become one single integrated problem.

2.1. Heuristic-based design

Over the years graphical and heuristic based methods have been proposed and used with high acceptance in industry. The reason is primarily practical; typically most chemical processes are rather complex, with a very large number of design options, and prior to the explosion of cheap personal computing it was simply intractable to deal with all possible combinations and decisions in a rigorous way (and still is in most cases). Therefore, the collective wisdom and experiences of practicing chemical engineers and researchers became collected in the form of very useful heuristics that allowed designers to quickly make decisions in complex situations that had a high probability of being practical, useful, and successful, although probably sub-optimal. This is particularly common in areas such as heat exchanger networks, water networks, process synthesis, distillation, intra-facility integration (i.e., "total site" integration), and inter-facility integration.

Some of the most common examples lie in the area of heat exchanger network design. This is a common process design situation in a classical process design methodology where a designer has synthesized the major portions of a chemical process (such as reaction and separation steps) but has not yet done heat integration. In this case, the locations and amounts of temperature/phase change steps are known in the process (e.g., this stream needs to be cooled by a certain amount at this specific point in the process), but the means for achieving this have not yet been

determined (e.g., either through intra-process heat exchangers or through the use of utilities). This is a complex optimization problem with both continuous and discrete decisions such as determining which streams should be matched, split, rerouted, etc., with complexity that increases combinatorially with the number of streams. Early attempts to address this problem include rules proposed by Masso and Rudd (1969) or Ponton and Donaldson (1974), to the addition of a thermodynamic approach to formulate the pinch method (Linnhoff and Hindmarsh, 1983).

Another example lies in water network design problems, which have similar challenges and structure to heat exchanger network design problems. Although some of the earliest works on water exchange network problems such as Takama et al. (1980) used a mathematical approach instead of a heuristic one, it proved to be too difficult to implement and solve given the technology available at the time and so was not widely adopted. Instead, heuristic approaches continued to be used for many years. For example, In 1989, El-Halwagi and Manousiouthakis (1989) proposed a targeting graphical method for mass exchange networks. A few years later, Wang and Smith (1994) proposed the so called "water pinch" for minimization of water consumption, following the example of pinch-methods in heat exchanger network synthesis.

Although heuristic methods gave way to mathematically-based methods (see next section) as computing power became more available, even the more modern mathematically-based methods still rely on the general process design methodology heuristic that the main process is designed without regard for energy/mass integration, and the heat/water exchanger networks are designed last. This philosophy is built directly into the AspenOne Engineering Suite, in which the process designer first creates the flowsheet model in Aspen Plus using "half" heat exchanger models that indicate how much a stream should change its enthalpy, but without considering the other half of the heat exchanger. The user then typically chooses either to integrate the half-sections manually or to use the now outdated MHeatX block to link all of the half-heat exchanger models together in order to create a (typically impractical and largely theoretical) heat exchanger network through a heuristics-influenced pinch-based algorithm. Although the newer optimization-based Aspen Energy Analyzer (AEA) replaces this, it still relies on the larger heuristic in which the process is designed first and the exchanger network second (Adams, 2017). The alternative is to synthesize the process and heat exchanger networks simultaneously, which is often too complex to be tractable.

This is why the two main approaches for process flowsheet synthesis still in use today place heat exchanger network design at the end. For example, the hierarchical decomposition method (Douglas, 1985; 1988) takes an iterative approach where the complete flowsheet is improved in stages, increasing the resolution of the flowsheet each time by replacing simplified models or sketches with more detailed versions until the full detailed picture emerges. Heat exchanger network design is the very last stage. The onion method bases process design around the synthesis reactor operation, by first focusing on the reactor stage in detail as the center of the onion, and then designing more layers around it by synthesizing and designing the unit operations increasingly further upstream or downstream from there until the raw materials and final products are reached (Smith, 2005). In this approach, the final layer of the onion is the design of the heat exchanger network.

Heuristic decisions made within both the hierarchical method and the onion methods have long been in use. For example, classic books by Seider et al. (2017) and Woods (2007) contain extensive advice on both flowsheet and unit operation design that rely on engineering wisdom, such as whether to choose expanders vs. flash valves, where to place pressure and temperature change equipment relative to other units, whether to transport materials as liquids vs. gases, which kinds of equipment to select, how

recycle streams should be incorporated, and many other decisions. Seader and Westerberg (1977), gave now well-known heuristics for distillation column sequencing, which for many years was the only practical way to approach distillation sequence problems that increase combinatorially with the number of chemical products being recovered, quickly rising to many millions of possible flowsheets. Other examples within process design include geometric rules for the selection of reactors and reactor networks (Glasser et al., 1987).

These same heuristic-based design principles apply also not just to the design of individual processes, but to the design of systems that integrate multiple processes together, called total-site integration. The objective is to exploit synergies between processes in large complexes in order to save utilities and resources (Klemeš et al., 1997), especially with the integration of intermittent renewable energy sources as they require more complex design considerations (Varbanov and Klemeš, 2011). Heuristics have even been proposed to integrate processes together even more tightly such that it is better called process intensification (Klemeš et al., 2014) where units, equipment, or process sections are shared between processes to reduce the total amount or footprint of the overall site.

Product design heuristics, however, were not a traditional focus of the process systems engineering community and so they are only discussed here briefly. Instead, they fell within the management science community (Kohli and Krishnamurti, 1987) until the work by Cussler and Moggridge (2011) that provided guidelines in a process systems engineering context. More recent examples include Arrieta –Escobar et al. (2018) who suggested a heuristic based methodology for the design of consumer products applied to cosmetics. The authors' own industrial experiences have shown that companies typically utilize their experts' know-how, years of experience, and wisdom to guide the development of new products. In almost all cases, overall, heuristic design approaches completely separate product design from process design.

2.2. Mathematical-based design

The development of mathematical-based methods runs in parallel with the development of solvers and computing power. Thus, mathematical-based methods began to replace heuristic methods for solving more and more complex problems (Grossmann et al., 1999). For the example of heat exchanger network design, early attempts using sequential methods to determine the utilities consumption, stream matches, and the network were not capable of resolving the trade-offs between operating and investment costs (Floudas et al., 1986), leaving the heuristic methods described in the previous section as the preferred method of the day. However, key mathematical improvements changed this, such as the development of simultaneous design approaches based on superstructure optimization (Yee and Grossmann, 1990), or pinch locator approaches (Duran and Grossmann, 1986). However, large scale problems involving entire flowsheets are still quite challenging. For example, sequential framework approaches are able to handle larger problems, but not prove global optimality (Anantharaman et al., 2010).

However, current algorithms are now effective and convenient enough that although global optimality may not be guaranteed, and simplification techniques may be required such as piecewise linear approximation of heat capacity relationships, they have effectively replaced heuristic methods in many cases. One example is the previously-mentioned Aspen Energy Analyzer which commercialized many of the theoretical and algorithmic developments listed here to make mathematical-based heat exchanger network design easily and rapidly available to non-experts. Although using the software requires some user input such as defining hot and cold streams and defining some user-level heuristics such as constraints on network complexity, even these inconveniences can potentially be replaced with the development of new algorithms such as the one presented by Quirante et al. (2018). This new algorithm updated Duran and Grossmann's (1986) method to automatically classify streams as hot or cold without need for user specification.

Water network design problems followed a similar history, having similar mathematical characteristics to heat exchanger network design problems. Like heat exchanger networks, early attempts at mathematical optimization for water management such as Takama et al. (1980) or Papalexandri et al. (1994) helped advance theoretical developments but were not widely adopted because of the difficulty in the solvability of the MINLP formulations. However, Galán and Grossmann (1998) revisited Takama et al. (1980) to solve a superstructure of all possible re-use and recycle opportunities, making major headway into the use of mathematical approaches by making the problem both generalizable and practical. This continued to be improved with key advancements such as the Karuppiah and Grossmann (2006) development of a spatial branch and contract algorithm for the rigorous global optimization of water system design that was updated by Ahmetovic and Grossmann (2011). This has made solving generalized water network synthesis problems mathematically much more practical and more widely adopted, even becoming an important benchmark test problem within the field of optimization itself (Teles et al., 2012; Misener and Floudas, 2014).

Now that optimization approaches to heat and water exchanger design are widely used, it is only natural that the next level of development include the integration of these two design problems together or even into other aspects of flowsheet synthesis and design. Key examples include simultaneous heat and water synthesis in a two-stage procedure by Grossmann and Martín (2010), a targeting procedure to simultaneously integrate water and energy integration by Yang and Grossmann (2013), and a procedure to integrate heat, water, and power together simultaneously within the process design (Baliban et al., 2012). These latter approaches are the next step in the path toward optimization approaches which incorporates more and more design decision-making into the optimization framework, and leaving less and less for the designer. These are the early indicators of the future directions of the field which we will discuss in later sections, as they are not yet adopted since the complexity barrier to the typical designer remains too high.

Within the space of process flowsheet synthesis and process design outside of heat and water networks, mathematical programming based approaches have long been in use. Early examples in the power and steam production systems category include simple MILP formulations (Papoulias and Grossmann, 1983) to similar approaches using increasingly more rigorous models for the calculation of the thermodynamic properties of the steam such as Bruno et al. (1998) or more rigorous turbine modelling Varbanov et al. (2004). Recently, Pérez-Uresti et al. (2019) developed MINLP formulations for 100% renewable-based power plants integrating biomass, waste, solar and wind energy for the production of power and steam. Early examples in reactor network synthesis include designing reactors by optimization of the reactor conversion, which considers the dynamics of the kinetics in the formulation (Achenie and Biegler, 1986). The link between reaction and separation led to considering both simultaneously in the formulation (Balakrishna and Biegler, 1993). In terms of separation, with distillation columns the most energy intense units in industry, a number of early works deal with the optimal sequence of columns to separate mixtures (Andrecovich and Westerberg, 1985), including heat integration among them (Floudas and Paules, 1988) as well as the rigorous design of the columns themselves (Viswanathan and Grossmann, 1993). More recent advances

focus on optimal multicomponent distillation sequencing with the possibility of non-traditional, thermally coupled sequence configurations, which explores a very large combinatorial space of possible designs in an optimization framework (Shenvi et al., 2012).

In all of these examples, the designer still employs a large amount of engineering expertise in order to define the optimization problems that will help determine the best unit operation parameters or flowsheet structure. For example, in order to have an optimization-based software approach for process synthesis, Kravanja and Grossmann (1990) developed PROSYM, currently renamed as MYPSYN (Kravanja, 2010). However, as is still commonly the case today, the "superstructure" (a description of all possible flowsheets should be considered as candidates for optimization) must still be modelled and defined manually on a case-by-case basis, which requires considerable process knowledge and expertise beforehand. New approaches, called automatic process synthesis, depart from this method and are gaining attention. In automatic process synthesis, either the superstructure subject to optimization is created by algorithm instead of by the designer, or, the chemical process is represented as a series of generalized interacting chemical phenonema rather than specific unit operations. Early attempts into this include Papalexandri and Pistikopoulos (1996) which use general representations of mass and heat transfer to describe a chemical process rather than pre-defined units. Later, Super-O was released as a package that considers the thermodynamics and physical properties of participating chemicals (Constantinou and Gani, 1994) in automated process synthesis Implemented by Bertran et al. (2017) so as to combine automatic reaction pathway synthesis, automatic products selection (as in the choice of the reagents or products themselves may be determined automatically), and knowledge databases of existing technologies and pathways into one tool which produces the superstructure topology and solves for the corresponding optimum process via GAMS, all managed through the Super-O user interface. Although this is a big step toward fully automated process synthesis, the human designer still plays an active role in engineering decision making and data collection throughout the process. Another competing and equally ambitious approach is that of Demirel et al. (2017) which uses a generic block and grid superstructure in which optimization is used to solve for the chemical phenonema that should occur in each block and how much matter and energy should be transferred from one block to another. Unit operations (i.e., the chemical equipment) are not directly determined, but rather they can be inferred directly from the phenonema that occurs within each block. In some cases, this could lead to suggestions of new unit operations that currently do not exist.

Design procedures that consider flexibility in production have only started to appear recently due to the complex models required (Martín and Martín, 2013; Grossmann et al., 2016; Peng et al., 2019), but have been extended to polygeneration systems (Adams and Ghouse, 2015; Chen et al., 2012) and "total site optimization", which is heat integration between different processes (Nemet et al., 2015). These works typically use an approach where each unit operation or piece of equipment is designed for one specific purpose or product in a process train committed to one specific possible product of a flexible process. Thus, each unit in a product train is either turned up or down (or off) depending on how much of that product is produced at that moment in time. In flexible polygeneration plants of this type, certain upstream components (especially relating to syngas generation) are typically shared by all product trains and so are perpetually at steady state. However, some recent work has looked at designing processes in which downstream chemical process equipment is "always on" but is used for different purposes depending on which products are being produced. For example, Adams et al. (2018) pro-

posed a design under uncertainty methodology for designing a set of distillation columns in a flexible polygeneration plant that are re-used for different purposes at different times during the plant's lifetime based on changing market conditions or various business decisions. The proposed methodology retains the use of rigorous distillation models and is able to achieve global optimality in a reasonable amount of time for typical size problems.

For years, design has been process-focused while product design was addressed as a separate problem. Typically, product design focused on molecular design (Gani and Brignole, 1983), catalyst design (Gounaris et al., 2006), and protein folding (Floudas et al., 2005) etc. for which global optimization became the driver via software like BARON (Sahinidis, 1996), sbb (Androulakis et al., 1995), and more recently ANTIGONE (Misener and Floudas, 2014). General packages for product design have been developed such as the VPPD Lab (Sawitree et al., 2015). However, sometimes there is special need to address process and product design simultaneously. Examples include the production of specialized ingredient-based products (Martín and Martínez, 2013,2018; Gani and Ng et al., 2015; Zhang et al., 2017), the production of fuels within environmental regulations which requires mixing or blending (Zhao and Wang, 2009; Guerras and Martín, 2019), product/process design related to separations (Eden et al., 2004), the design of algae for fully renewable biodiesel production (Martín and Grossmann, 2013), the design of specific molecules with a desired properties (i.e., reactant media Struebing et al., 2017; solvent selection, Gopinath et al., 2016), and addressing process design considering product characteristics (Moggridge and Cussler, 2000; Gani, 2004).

2.3. Hybrid approaches

In most cases the actual number of technologies is so high that it makes sense to follow a two-stage evaluation procedure to discard those less promising due to their early stage of development or the extreme costs (Guerras and Martín, 2019). In a second stage a superstructure of alternatives can be put together (Martín and Grossmann, 2011). Alternatively, if the number of alternatives is small, a scenario-based approach can be performed using rigorous process simulators (Zhang et al., 2013). Finally, stochastic optimization using process simulators can be employed to take advantage of detailed models of distillation columns, liquid-liquid extraction columns, and other models that are implemented in rigorous process simulators (Adams and Seider, 2008). However, the optimization time increases exponentially with the number of degrees of freedom, and global optimality can almost never be guaranteed. Furthermore, reactors are not typically addressed very rigorously (i.e., Ramírez et al. 2018).

3. Challenges in process and product design

Fig. 1 summarizes the grand challenge of chemical process and product design. The problem boils down to determining what products will best suit customer needs, and then creating a process to produce them in an optimal fashion from certain resources and raw materials. The key decisions are usually related to the choice of unit operations and their operating details (size, shape, pressure, temperature, flows), the selection and pre-treatment of raw materials or feedstocks, reaction conditions and reactor design, separation and purification system design, recycle streams, temperature management, pressure management, utility selection, and the handling of wastes, including heat and water recovery. Optimality is usually characterized by economics or business objectives (such as maximizing profitability or net present value, minimizing cost, minimizing utility consumption), minimizing wastes, minimizing environmental impact, or combinations of these. Although this has
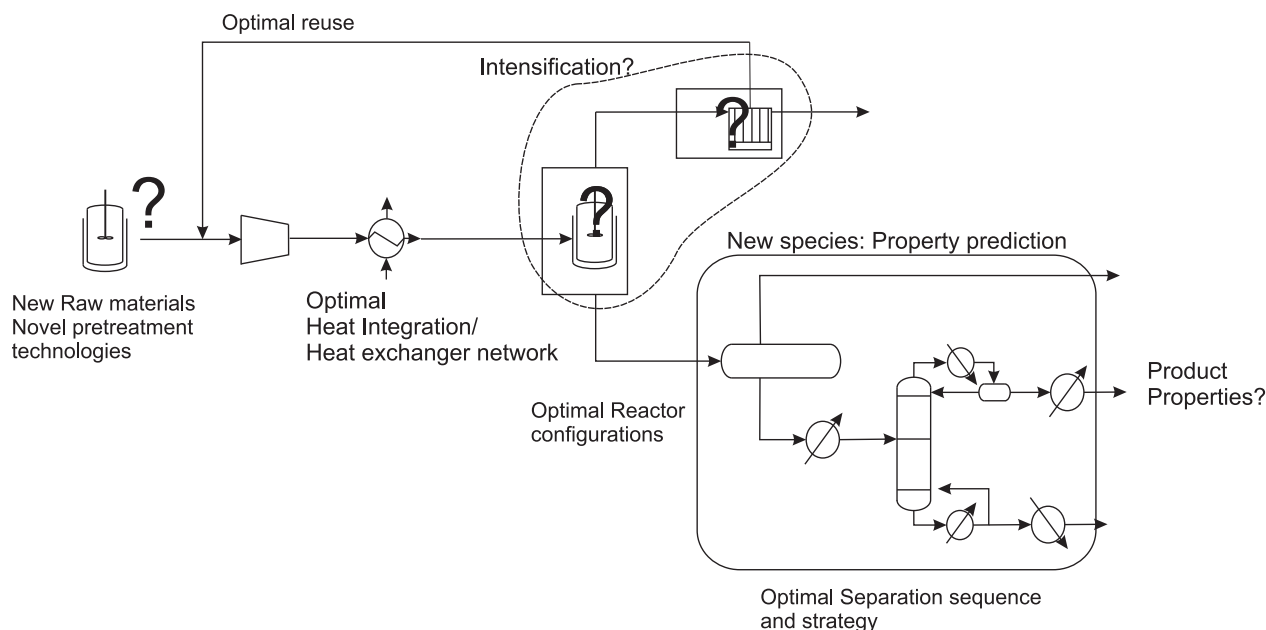
Fig. 1. Challenges in process and product design.

always been the focus of the process designer, several new challenges have become particularly important.

3.1. New sources and products

The recent focus on environmental concerns for the chemical industry has brought several new potential feedstocks to the forefront. These especially include biomass and wastes as a source for power and chemicals and the use of CO_2 as carbon source and as a means of carbon disposal for climate change mitigation. Thus, the circular economy concept for the reuse of waste has become an interesting trend as a way towards reducing the exploitation of natural resources by providing a more efficient use of them (Korhonen et al., 2018). Another important link is the one involving water, energy and food, resources that lie at the foundations of life and are thus some of the main pillars of our society (García and You, 2016). As a result, a number of residues for different activities such as agricultural, food industry and even heavy industry have become raw materials, not only in the form of mass residues but low temperature sources of heat. Furthermore, energy from nuclear, solar and wind can be used either to displace fossil-based electricity consumed in chemical plants, or, be used to drive chemical conversion processes (such as through electrochemical conversion or as a heat source) (Scott and Adams, 2018; Hoseinzade and Adams, 2019). However, the variability of renewable sources greatly impacts process design (Martín, 2016a, b) and operation (Zhang and Grossmann, 2016). For example, optimization under uncertainty plays an important role to evaluate the effects of resource availability on unit size (Pistikopoulos and Ierapetritou, 1995). Two types of uncertainties are found in these processes: exogenous, which is based on the uncontrolled variability of the resource (Martín, 2016a, b), and endogenous, which is the uncertainty in yields based on potentially immature technology (Gupta and Grossmann, 2014). However, optimization under uncertainty problems are complex and require novel solution procedures (Lara et al., 2018; Heuberger et al., 2017).

Similarly, new environmentally-motivated products are now of interest too, such as biodiesel from different alcohols, glycerol ethers (de la Cruz, 2014), biobutanol as a gasoline substitute (Dalle Ave and Adams, 2018), bio–butyl butyrate as a jet fuel substitute (Birgen et al., 2016), and dimethyl ether as a diesel substitute (Ballinger and Adams, 2017; Martín, 2017) or the production of bulk chemicals from alternative resources including methanol (Martín, 2016a, b, Martín and Grossmann, 2017a, b) or ammonia (Pfromm 2017; Sánchez and Martín, 2018). Furthermore, advanced and high added value materials from waste and biomass are the key for economically promising bio-refineries. Polymers such as a polyesters, polyhydroxybutirate (Bueno et al., 2015), drugs, proteins, and carotenoids (Psycha et al., 2014) have been produced out of renewable sources including algae or lignocellulosic biomass. These new materials are great examples of the link between process and product design by targeting the properties that meet society needs, which is made possible by good physical property estimation models (Marrero and Gani, 2001).

Research in this area, particularly with regards to biomass, is quite active. There are very many proposed process concepts which on paper appear to be very promising. One of the primary challenges for the field, though, is advancing the concepts far enough to actually become commercialized, as concepts such as large complex bio-refineries have yet to be adapted seriously. Many of the key barriers are economic, as the business-as-usual ways of producing chemicals and fuels from traditional sources are typically much more profitable, whereas many alternative routes using renewables may even require a significant government mandate or incentive to be economically viable, which in turn imposes a societal cost. Linked to this, therefore, are significant uncertainties in future government policies and social support which are magnified in any project that depends heavily upon them. Equally important are logistical factors involved in large capital projects involving renewables, where the variability of the feedstocks or energy sources are far beyond what the bulk chemicals industry is used to managing but are a major complication.

Process designers can help assuage these issues by considering these issues more directly in their designs. For example, processes which have built-in flexibility in product or reagent (as discussed in later sections) may be able to provide a better economic case for renewables integration by creating processes which are robust to major uncertainties such as markets, availability of renewable

resources, and changing government policy. In other cases, the best approaches will be to bring costs down for the larger business as a whole by considering the design in the larger framework of supply chains, planning, scheduling, operations, and public policy.

However, an equally important consideration is that chemical process designers can do a lot better job of communicating their results with each other and with the public at large. There are hundreds or thousands of studies that show potential alternative processes that use some newer renewable energy source like biomass as a key component. Nearly each study published in this area concludes that whatever concept was presented is promising and worthy of consideration or construction, and yet almost none have been commercialized. One big reason for this is that it can be very hard to determine the best and most promising technologies amongst all of the noise and hype. Therefore, one of the most important future directions of the field in this area may be to conduct meta-studies that critically examine the field of proposed process designs in the literature within a common set of assumptions and standards in order to make decisions about which processes are the most promising. Such studies would be very valuable in order to identify the most promising new pathways to include renewables. This would in turn inform researchers, policy makers, and funding agencies to help focus research on the most promising areas and allow their benefits to be achieved more rapidly.

3.2. Novel technologies

The use of alternative sources of energy and chemicals leads to the development of novel technologies to process them. In brief, from the process point of view, we highlight catalysts, since they will allow the chemistries providing a larger yield and selectivity to the desired product/products. These catalysts are used in reactors that also present challenges related to their structure for proper mass and heat transfer. Particular cases are bioreactions. They are limited by the poisonous nature of the products on the catalyst, the enzymes, and the need for cooling while operating at low temperature. Furthermore, heterogeneous catalysts, although can reduce purification stages, show mass transfer limitations too. In terms of separations, novel production processes typically show more complex purification schemes where efficient units, i.e., divided wall columns, reactive columns, or membranes should be the key for a sustainable production. We can envision a number of challenges:

1. The large community in different fields evaluating the use of more sustainable resources results in a number of alternative technologies to process the raw materials into the products that must be screened before detailed process design is attempted. The efficiency of these technologies may also be resource dependent.
2. New units involve complex or not-well understood mechanisms. Moreover, the presence of biological material involves the difficulty of living systems. This is also a source of uncertainty, and much experimental work is being carried out to understand living systems.
3. Apart from living systems, the thermodynamics of the novel products and mixtures determine the design of any single unit. These can introduce complexities such as azeotropes and liquid-liquid equilibrium as in the production of biobutanol (Malmierca et al., 2017), to particle-based operations that involve mass and energy transfer.
4. The scope of the chemical process systems designer is getting larger, requiring knowledge outside of the boundaries of classical process systems engineering or even the whole of chemical engineering. To solve modern large-scale problems, systems engineers must often incorporate aspects of biology, chemistry,

logistics, agriculture, business acumen, high performance computing, climate science, economics, medicine, physiology, socio-political considerations, and even marketing into the design process. This is a challenge for the process engineers due to the need to learn the language of a number of other specialists becoming a facilitator between scientist and technologists.

3.3. Process modelling

Process design requires a large amount of chemical process modelling in order to adequately consider the fundamental thermochemical principles involved. Furthermore, modelling novel technologies is challenging due to the lack of data and fundamental understanding of the phenomena involved. Typically, the plant design is carried out using limited data including experimental results at lab scale (Martín and Grossmann, 2012), and thus the models inherently have a certain degree of uncertainty. However, it is essential to have a good understanding of each unit operation in order to develop predictive models that facilitate process synthesis and permit meaningful analyses of its performance within this uncertainty without having to construct the actual plant.

A number of approaches for developing good models have been used over the years. First principle models are the most commonly used, which are models that are developed from the first and second laws of thermodynamics, and typically include aspects such as mass balances, energy balances, and momentum balances of which there is well-known underlying theory. These models also incorporate models of the underlying physical properties of chemicals and mixtures, such as valour-liquid equilibria, state variable relationships (i.e., equations of state), thermochemical properties such as heat capacities, densities, and surface tensions, and reaction behaviour such as equilibrium and rate-law kinetics. These physical property models are usually determined empirically from experimental data (perhaps fitting parameters to a model equation that may or may not be based on theory) and are commonly available to researchers.

The first principle model approach is very convenient because it allows one to create models of a wide variety of chemical process units in almost unlimited number of applications (Martín and Grossmann, 2012). These models can be customized according to the level of rigour and complexity required, ranging from simple "zero-order" steady-state models of a process unit to detailed dynamic models with millimetre spatial resolution in three dimensions, and they can be applied to applications at scales large and small. For example, we can find computational fluid dynamics (CFD) models for reactors or spray driers (Hernández et al., 2017, Portillo et al., 2007), Discrete element methods (DEM) models for particulate based process (Hassanpour and Ghadiri, 2015), multi-phase reactors (Dudukovic et al., 1999), rigorous models for distillation columns, adsorption columns (i.e., Ramírez et al. 2018), and detailed models for reactors (i.e., Adams and Barton, 2009, Hoseinzade and Adams, 2017). These individual models can then be conveniently interconnected to form a flowsheet model of an entire process. Since models of this type are often generalizable, they are often compiled into libraries and made available for distribution and use with process simulators like ASPEN Plus, ASPEN Hysys, ProMax, Pro/II, CHEMCAD, gPROMS, or Jacobian. They key challenge, however, is that detailed experimental data are rarely available for each specific individual unit of interest in a process, let alone for an entire process, since the goal of conceptual process design is often to design processes which have not been created yet. However, because the underlying models are based on first principles with the backing of experimentally-derived parameters, they are still useful and meaningful for process synthesis and analysis.

An alternative approach to using first principles models is to use data driven models, which are starting to be widely used in the process industry (Boukouvala et al., 2010). For example, instead of using first principles, key unit operations (or entire process sections) can be modelled purely from the collection of experimental data of that process. This data can then be used to create data-driven models of many forms in which typically contain equations and tuning parameters which are only useful to that specific application and are not generalizable to other contexts. These data-driven models can be created using techniques such as latent variable multivariate regression (Burnham et al., 1999), principle component analysis, partial least squares regression (Westerhuis et al., 1998), artificial neural networks (Eason and Cremaschi, 2014) and other "machine learning" type approaches. Surrogate model approaches (Caballero and Grossmann, 2008; Henao and Maravelias, 2011; Cremaschi, 2015; Ma et al., 2016; Bhosekar and Ierapetritou, 2018; Schweidtmann and Mitsos, 2019) such as those used by the software ALAMO (Cozad et al., 2014) can also be used to create data-driven models, although their primary purpose is to use a complex first principles model as the "true" process in order to create a reduced or simplified model for improve computational tractability. The advantage of data-driven models is that they are generally more accurate than a first principle model because it implicitly incorporates all phenomena involved, including hidden, unknown, or ignored phenomena that might not be incorporated into a first principles model. The disadvantages and key challenges include the large amount of data required to produce and validate the model, as well as the limited predictive capacity of the model outside of the range of the underlying experimental data. Thus, data-driven models are often better suited for model development of very specific and already-constructed units.

Although many algorithms, methods, and in-house tools have been developed or proposed which incorporate many mathematical modelling and programming advances for process modelling, many of these concepts remain out of reach to the average user. In general, the amount of effort and knowledge required to employ them, particularly with regard to computer programming needs since many of them may need to be custom-programmed by the process designer, outweighs the benefits for the typical industrial user and thus remains a major barrier to commercial adoption. In addition, even where individual algorithms or tools have been made available to the public or commercialized, they exist in a disjointed collection of individual codes which ultimately must be linked to and integrated with other codes, software, and frameworks from completely different authors or sources in order to make them the most useful. One ambitious project, called the Institute for the Design of Advanced Energy Systems' PSE Framework (a.k.a. that IDEAS PSE Framework), is being developed by the US Department of Energy's National Energy Technology Laboratory. At present, it exists mostly as a collection of open (free) process models for steady state or dynamic simulation, within a framework that is intended to facilitate the incorporation of advanced algorithms and tools such as advanced optimization, parameter estimation, and other features (Okoli et al., 2018). Although the modelling capabilities are limited compared to commercial flowsheet software, the most promising feature is the unified framework on which it is built. On this platform, future features may be built by third-party developers and academics, facilitation more rapid user adoption. However, making these advanced methods more accessible and convenient remains a major practical challenge for the field today.

3.4. Electricity and energy storage

Chemical process engineers have rapidly moved into the field electricity generation processes. Although electricity generation was traditionally the domain of electrical and mechanical engineering, the interface between electricity and chemical production has become increasingly important. Commonly, this link occurs as a waste handling step in chemical production, in which high-energy off-gases from a chemical process used as fuel for a power plant in various ways, leading to polygeneration processes (Adams and Ghouse, 2015) or simply the chemistry and thermodynamics involved in combustion of different raw materials, the use of hot brines and the thermodynamic cycle, Brayton and/or Rankine involved in the transformation of the thermal into electrical energy (León and Martín, 2016; Peña et al., 2018). However, because electric power production is driven by demand, and because electric grids are increasingly dependent on renewables in which power generation cannot be controlled, there is a clear mismatch between production and consumption. Grids with limited amounts of renewables traditionally handled this mismatch by raising or lowering natural gas combustion rates in response to demand. However, more modern grids with large amounts of integrated renewables face a new problem in which more electricity is produced than consumed, despite shutting down all natural gas peaking plants. This leads to a modern problems associated with electricity disposal, which is sometimes resolved by selling it at negative prices (Dowling and Zavala, 2018)

A number of chemical engineering solutions have been discussed to address this issue. To mitigate the temporary absence of a resource, the integration of several of them provides backup (Yuan and Chen, 2012). However, process and resources integration are not enough. Thermal or chemical storage of excess energy generated by renewables is increasingly of interest. For example, concentrated solar power plant designs have proposed thermal storage options, i.e., molten salts, in which heat from solar power is stored as hot water or waxes (Slocum et al., 2011; Martín and Martín, 2013), and chemical storage options, in which heat is used to drive a reversible endothermic reaction such that energy is stored as chemical potential (Lai and Adams, 2018). In either case, the idea is to run the system in reverse to generate heat for steam production when power is needed. While these addresses day-to-day variation, seasonal variation might be better dealt with by integrating solar energy with biomass combustion during less sunny months (Vidal and Martín, 2015), since biomass is how nature already stores solar energy. Instead of thermal pathways, electrolytic pathways can be used to create H_2 from water via electrolysis when extra electricity is available. When combined with CO_2, high energy products such as methane, methanol, DME, (Davis and Martín, 2014; Martín, 2016 and 2017) or polymers (von der Assed and Bardow, 2014) or ammonia (Sanchez and Martín, 2018) can be produced, thus storing the energy in fuel form. Physical pathways are also possible, in which excess energy (electricity or mechanical work) is stored by compressing a fluid such as air (Nease and Adams, 2013).

The biggest key chemical engineering challenges within energy storage lie at the intersection of cost, scale, speed, and reliability. For example, classic electrochemical batteries are reasonably affordable for many common household applications, have very fast demand-response times, and are quite reliable. However, they do not scale well for large energy applications, which is where the chemical solution may be best. The challenge, though, is to create thermochemical energy storage which are able to achieve high performance, reliability, and low cost at the relevant scales. Fast demand-response performance is potentially the most difficult, as energy storage systems that rely on classic chemical technology are likely to be far too sluggish to match the near-instantaneous response of batteries, flywheels, and supercapacitors. It is more likely that chemical storage systems will be hybridized with electronic ones in which the batteries and supercapacitors provide fast demand-response in smaller amounts while chemical energy stor-

age provides affordable longer-term storage at scale. The challenge is identifying and designing the right systems for the right niche applications.

3.5. Process intensification

Process intensification has played an important role in the efficiency of processes by reducing the size of individual pieces of equipment, the number of unit operations involved, the wastes and unwanted byproducts, and the energy and water consumption. Process intensification departs from classical chemical process design because in classical design, one typically creates the process from a collection of standard pieces of chemical equipment (pumps, compressors, reactors, heat exchangers, binary distillation towers, etc.) that are linked together by streams and pipes, typically without regard for physical space or land area occupied. Process intensification turns this on its head and focuses instead more at the unit operations and thermochemical phenomena level. The key idea is that while classical chemical technology is generally designed to do one specific task, it may be better to design new kinds of chemical equipment that are optimized for multiple tasks together in the same device. Although intensified processes can be more challenging to create, more complex, and less generalizable, the benefits often are reduced capital expenditures, reduced space footprints, reduced operating costs, and reduced environmental impacts.

One of the most commonly cited examples of successful process intensification is the dividing wall column (Dejanović et al., 2010). For systems of three or four components that must be separated by distillation, the classical approach is to use a series of binary distillation towers, which is still quite common. This approach is fundamentally inefficient because the first binary column of a column series does the work of partially separating the three or more components in the feed before remixing them into just two products (distillate and bottoms), which wastes the energy spent on that partial separation. For example, for a feed containing A, B, and C, suppose A is collected in the distillate and B and C are together collected in the bottoms to be sent to a second distillation column. In this case, the concentration of B is higher on the trays in the middle of the column, because it has been partially separated from the B and C, only to be remixed with C as it falls down toward the bottom. The Kaibel prefractionation approach solves this problem by having a prefractionation column that partially separates the feed into rough AB and BC cuts before the main column, and the process intensification aspect is that it receives its liquid and vapour "reflux" streams from the main column, rather than through its own condenser or reboiler. The dividing wall column further intensifies this by locating the prefractionator inside the same shell as the main product, as they describe in their patent (Kaibel et al., 1993).

Other examples of process intensification include multifunctional reactor for biodiesel production (Harvey et al., 2003), reactive distillation (Segovia-Hernández et al., 2015), energy-coupled columns (Caballero and Grossmann, 2013), internally heat integrated distillation columns (Kiss and Olujic, 2014) and semicontinuous distillation (Ballinger and Adams, 2017). These reduce the size, weight, number of process equipment, and/or energy consumed by finding clever ways of combining multiple fundamental operations into the same space. The integration between membrane separations and distillation has recently been applied to overcome thermodynamic limits such as azeotropes (Lutze and Gorak, 2013) or to improve the conversion using membrane reactors (i.e., Assabumrungrat et al., 2003). However, membrane material evaluation and design is still a field in development.. Furthermore, intensification has been evaluated in the integration of renewable energy with traditional resources. Particularly interesting has been the intensification of processes using solar energy (Gençer and Agrawal, 2017; Vidal and Martin 2015) as well as for thermal energy storage (Guo and Goumba, 2018).

Another trend related to the use of renewables and its distributed production is modularization. The concept of modular design is that cost savings are achieved by designing a collection of prefabricated unit operation subsystems that can be readily "mixed-and-matched" to create new kinds of unit operations. In this way, future process designers would create unit operations out of well-known and understood standard subsystems in the same way that current process designers create processes out of well-known and understood standard chemical equipment. The modular units would be pre-fabricated off-site and designed for quick integration and installation, thus yielding savings both from reduced custom design costs and from the resulting intensified process (Bielenberg and Bryner, 2018). However, the main challenges lie in the high risk of failure, the lack of scale-up knowledge, and safety issues (Kim et al., 2017), as well as their general complexity.

Although the concept of process intensification has been at the forefront of research, such as the interesting overview by Stankiewicz and Moulijn (2000), it has not actually achieved widespread adoption. Traditionally, intensification has generally been carried out through expertise, based on specific examples and circumstances. Because of this, many process intensification cases can be one-off type situations, where the costs and risks of developing a new and individual piece of equipment may be very high compared to the ease of using very mature and well known technologies, despite their inefficiencies. The most commercially successful examples cited above (dividing wall distillation and reactive distillation) are ones in which the benefits of intensification are general and not case specific. The benefits of intensification in those cases arise because the original approach is fundamentally and obviously thermodynamically inefficient, and perhaps in hindsight we never should have been doing that to begin with. However, most intensified designs do not generalize this well, and as such, there has been a lack of the development of software, tools, education, and expertise, which has stymied the commercial adaptation of process intensification in general (Bielenberg and Bryner, 2018).

The main challenges, therefore, are to create the necessary tools, expertise, and educational resources that enable designers to more rapidly and cost-effectively approach process intensification. This requires approaches that look at chemical processing "outside the shell" of each unit operation and instead focus on specific chemical phenonema and driving forces rather than unit operations. Some of the more promising approaches include the more generalized flowsheeting approaches for process synthesis of Baldea (2015) which can help identify process intensification opportunities, as well as the generalized phenonema-block structure approaches of Demirel et al. (2017). Although these tools are still largely in-house, they could form the backbone of widely-adopted commercial tools to facilitate more rapid adoption. Other challenges include expertise, education, and changing the prevailing chemical engineering design ethos to think at the level of individual chemical phenonema when designing flowsheets. For example, process intensification concepts and thinking could be better incorporated into undergraduate courses in chemical engineering in areas such as separations, reactor design, and process design.

3.6. New targets and metrics

Economic objectives have been the obvious choice for characterizing plant quality, and most heuristics and rules of thumb in the chemical industry have been developed with this in mind. However, they are no longer socially acceptable in a more conscious world aiming at sustainable solutions. Now, a second objective is

environmental impact minimization. There are a number of metrics (i.e., GREET, TRACI, ReCiPe) that measure the impact generated by a process, with life cycle analyses the most common technique for obtaining these metrics to be used in process optimization (Kniel et al., 1996; Azapagic, 1999). There are many different environmental metrics which can be considered, such as climate change potential, smog forming potential, resource depletion, water consumption, toxicity to humans or wildlife, and acidification. Often these metrics are difficult to compare directly to each other on a quantitative basis.

More recently, social issues are now being included as decision making criteria within the design process. For example, the Jobs and Economic Development Impact model (JEDI) developed by the NREL can estimate the economic impacts of constructing and operating chemical and power facilities, which can be included in process synthesis (You et al., 2012). Safety has also been included as objective, although the concept dates back to work by Klenz (Klenz, 1984). These concepts have been included in process synthesis as another objective (Ruiz-Femenía et al., 2017) and for the selection of heat transfer fluids, within the new simultaneous process and product design paradigm (Martínez et al., 2017).

The optimal design problem is now largely multiobjective. Dealing with a large number of metrics is not easy and sometimes they are interrelated, correlated, or difficult to compare. Several strategies have been used, either by producing a single-weighted objective function such as ecoprofit (Cucek et al., 2012) or RePSIM (Martín, 2016b), or by using a constraints-based approach. Other work has been proposed on methods to reduce the number of objectives without eliminating solutions of the problem (i.e., Pozo et al., 2012). Alternative solution methods and metrics are required to better understand the solutions, for instance, evaluating the target yields of a particular technology for it to become competitive and enter the market and/or the energy mix, (Limleamthong et al., 2016; Ewertowska et al., 2016).

4. Near-term future directions

After this brief overview on process and product design and how they came to be evaluated simultaneously, we present some visions on the future of this field within process system engineering, focusing on areas that are still not very well studied within the field. Fig. 2 shows the interrelationships among various fields within process system engineering and how they are connected more than ever for a more sustainable industry.

4.1. Big data approaches to process and product modelling

Modelling is now the root of rigorous process and product design, often striking a balance between model rigour and model speed or complexity. While traditionally, first principle models and empirical correlations have been used for this purpose, the availability of data gathered in labs, pilot plants and industrial facilities is changing the approach. Machine learning to create data-based models is growing in popularity. Examples include estimating product properties and performance (i.e., wine taste, appropriate smell), which may not even exist yet. Given the more recent inclusion of social objectives, data and theory from outside engineering (including social science) will need to be included in big data approaches for product design. Artificial intelligence (AI) approaches will also become more in use, such as training artificial neural networks (ANN) to recognize heuristics and trends in human-designed processes and then use that to create new processes from the ANN models. For example, IBM's Watson platform is being trained with data from engineering operations documentation in order to make models of oil production operations. Engineers can ask plain language questions to get information about day to day operations or get suggestions on how to deal with problems as they appear (Lewis, 2017). Although not used for design currently, the same approach could be applied with an appropriate data set.

4.2. Process operation: integrated scheduling and operation

As discussed previously, one of the major trends within the field is the study of processes which directly incorporate renewable energy into it. The key challenge is that renewable energy sources such as wind, solar, and biomass, are intermittent, cyclic, dynamic, and uncertain, but with some degree of predictability at various time scales ranging from hours, days, seasons, and years. This means that the renewables-integrated chemical processes of the future will need to be designed taking all of this into account. With this kind of predictability, it is both possible and necessary to incorporate aspects of planning (long term) and scheduling (short term) methodologies directly into the process design. And, linked to that, how the process will be operated in response to changing
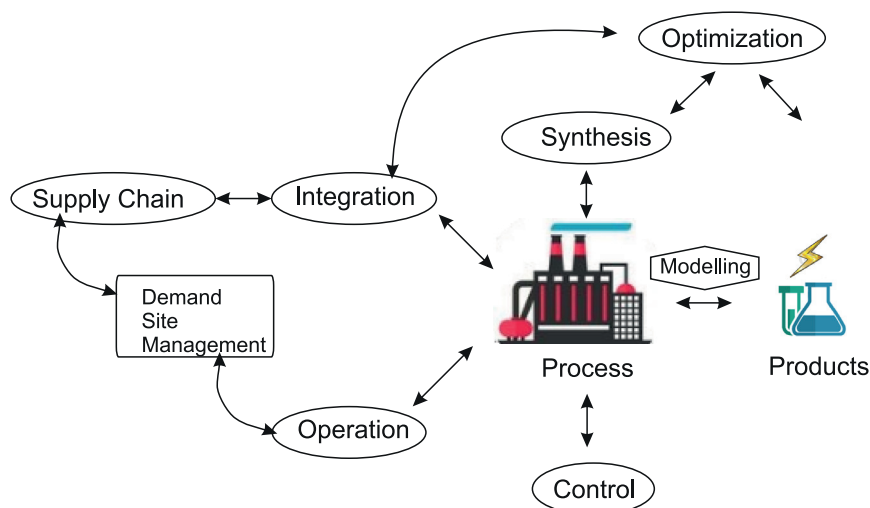

Fig. 2. Simultaneous process and product design.

renewable energy inputs (Grossmann and Guillen-Gosalbez, 2010). This means that in order to design a complex process using a large degree of intermittent renewables, the design procedure should be conducted simultaneously with planning, scheduling, and operational considerations, all wrapped within the context of optimality. The end result would yield an optimally designed process, along with the specifics of how to operate it in the face of changing renewable energy inputs, and the details of how to best plan and schedule for the impact of renewables.

This is a large problem, but one that is likely to become more important in the future. Some progress has been made in certain areas. For example, demand-side management is starting to address this issue with the integration of processes and their operation (Zhang et al., 2018). However, key challenges include the problem size, the various time and spatial scales involved, and understanding dynamic process characteristics and operation such as start-up and shut down (Baldea and Harjunkoski, 2014). Novel approaches are needed to address these problems (Pattison et al.). This is especially prevalent with systems that include energy storage technologies such as batteries, thermal fluids and chemicals, in which technology degradation over time becomes an important factor.

4.3. Process control

The use of renewable resources poses a challenge on the process controllability. The variability in the available resources of energy required not only careful planning but also demands more on the control structure of the process. In some cases, a way to mitigate the variability in the solar and wind energy when aiming at meeting a demand has been the integration of resources. Furthermore, integrated process design and control has been growing in popularity. The focus has been on the creation of a more robust or profitable steady state design and control system by considering the inherent controllability of the design in the face of uncertain disturbances (Ricardez-Sandoval, 2012; Washington and Swartz, 2014). In a renewables-driven process, uncertain disturbances such as minute-to-minute wind velocity fluctuation can be incorporated under this framework. On-line optimization using forecast of the weather data for the operation of energy systems has also been addressed (Zavala et al., 2009). However, more predictable disturbances (such as seasonal solar and biomass cycles) are better considered in an integrated design, control, and scheduling framework, which is at its infancy (Pistikopoulos and Diangelakis, 2016). Again, the dynamics of the systems plays a major role in these areas as well as handling uncertainty (Lubin et al., 2011). Intensification, described in Section 3.5 as a way towards energy savings, also required further work on the controllability of the intensified units due to the augmented complexity.

4.4. Supply chain management

Although the process designer generally assumes that resources will be available on demand, only larger scale supply-chain studies can provide insight as to how the process fits into the bigger picture. Renewable resources and, for example, biomass show additional challenges since the plant size is related to the amount of biomass that can be collected in a region (Marvin et al., 2012) and economies of scale that have been widely used in the chemical industry present limitations. Furthermore, it is critical to have a good understanding of the supply chain of a process in order to understand its true cradle-to-customer environmental impact. Thus, the design of the supply chain becomes directly linked to the design of the process when environmental considerations are made. In addition, in order to design processes which need to be flexible and reliable in their products, or use unreliable feeds (biomass in partic-

ular), one needs to be informed by their supply chains (You et al., 2012) towards mitigating the risk in the operation of the renewable based system (You et al., 2009). Either way, the link between process design and supply chain design will become increasingly important in an environmentally conscious world.

4.5. Computer science

Nearly all of the future directions put forward in this paper, from process modelling advances to integrated supply chain management, create mathematical problems which will require novel algorithms to solve. Efficient decomposition algorithms, modelling approaches, as and better software (or a combination of each) will allow us to solve larger and larger MILP or MINLP problems. Global optimization, despite its many advances, is still limited to small problems. Many of the future directions put forward in this paper are rooted in the solution of ever-larger problems with more complex models in order to capture and exploit more nuances and characteristics of the system. This means including more detail, non-linearity, and non-convexity, and so global solvers will need to be extended and improved. However, as engineers, a suboptimal solution is better than none, therefore solvers that handle large problems (but not guarantee global optimality) will be a necessary tool for practical process synthesis and operation. These include stochastic, evolutionary, or non-deterministic optimization algorithms which may not be elegant or theoretically attractive, but are undeniably useful.

4.6. Open access models, model sharing, and reproducibility

Although conceptual chemical process design and process systems engineering in general relies heavily on the use of models, it is rare that the models used to perform research, design processes, or analyse them are made available to other researchers. For example, a recent review of over 300 modelling and simulation studies within the field of energy systems found that just eight (!) made their models available to the public (Subramanian et al., 2018). Although many other fields of science routinely make their models and source code available to the public, this is clearly rare within the process systems engineering community. This unfortunately makes the research opaque and extremely difficult to reproduce.

For example, consider a typical conceptual process design and techno-economic analysis study in which the flowsheets of the process are drawn and briefly described in the text, but the underlying models (e.g., Aspen Plus files, GAMS code, Matlab scripts, etc.) are not provided digitally. The time for someone to reproduce the work from the publicly available information can sometimes take six months to a year, and that is only if the work provided a sufficient level of detail at every possible decision point. For processes with a hundred unit operations, it is nearly impossible to reproduce perfectly. Similarly, it is often impossible to judge the accuracy of the model implementation because it cannot be inspected by peer reviewers or the community in general. This adds a level of scepticism to virtually all research within the process systems community because one mistake in the development of a model can lead to meaningless results.

Therefore, the Adams group at McMaster has created the Living Archive for Process Systems Engineering, or LAPSE (see Fig. 3), which aims at providing a framework for the distribution of models, source code, software, pre-prints, and other open-access data within the systems community. Available at PSEcommunity.org/LAPSE, the archive has already received over 1000 submissions since its launch at PSE 2018, and has the financial support of the Computing and Systems Technology division of the AIChE, the Canadian Society for Chemical Engineering, SINTEF Energy, the

Fig. 3. The Living Archive for Process Systems Engineering at PSEcommunity.org/LAPSE.

Computer Aids for Chemical Engineering (CAChE) Corp., and the Technical University of Denmark. It also is officially partnered with the open-access journals *Energies* and *Processes* as a host of both models and open-access papers, and we openly encourage other journals to participate. We strongly encourage you to upload your models and source codes (or even sanitized versions for the case of models containing intellectual property such as with industrial collaborators) to LAPSE, and link to it in your papers. We believe this will greatly enhance the rate of progress of conceptual process design research, increase the reproducibility and accuracy of our work, and lead to greater global impacts. In fact, the most viewed submissions on LAPSE are those which contain open models, with the most viewed item on the website being an Aspen Plus model with over 1000 views.

One of the key goals of LAPSE is to better interconnect the different aspects and outputs of academic research to a broader community of stakeholders. The record maps feature (Fig. 4) allows a user to connect their submission to other submissions within LAPSE as well as material outside it (currently anything with a Document Object Index, or DOI). For example, a submission for a model might be linked to a (paywalled) journal article describing or using the model, a (free) pre-print version of that same manuscript, a conference presentation slide deck or video explaining or demonstrating the work, and links to research by other people that served as important pre-requisite knowledge or works that

derived from the current one. This helps to make the research more accessible to others, including non-academic stakeholders, because a visitor will come to the LAPSE record for one reason and be presented with an easy to understand conceptual map of how this work is placed in context with respect to other works, with immediate clickable access to them. Overall, this should elevate the field as a whole and increase its impact on the world in general.

In Fig. 4, a record map in LAPSE shows how the current submission (a preprint of a manuscript, with LAPSE tag 2018.0133) is related to other works. In this case, there are sibling works that include the final publisher's version of the paper, and software or source code that was used to help conduct the research described in the present record. LAPSE records also support links to child works that derive conceptually or depend on the present submission, or parent works from which the current work was derived. In this case, an Aspen Plus model (LAPSE:2018.0126) stored within LAPSE is a child record of the pre-print, and a conference presentation (LAPSE:2018.0398) is child of that model. Screen capture from http://PSEcommunity.org/LAPSE:2018.0133.

However, although LAPSE provides a technical means to foster model sharing, it will not be successful without a cultural change in the PSE community. Although many other academic communities have a culture of open model sharing, we simply do not. Fortunately, the tide is changing as evidenced by the rise of open ac-
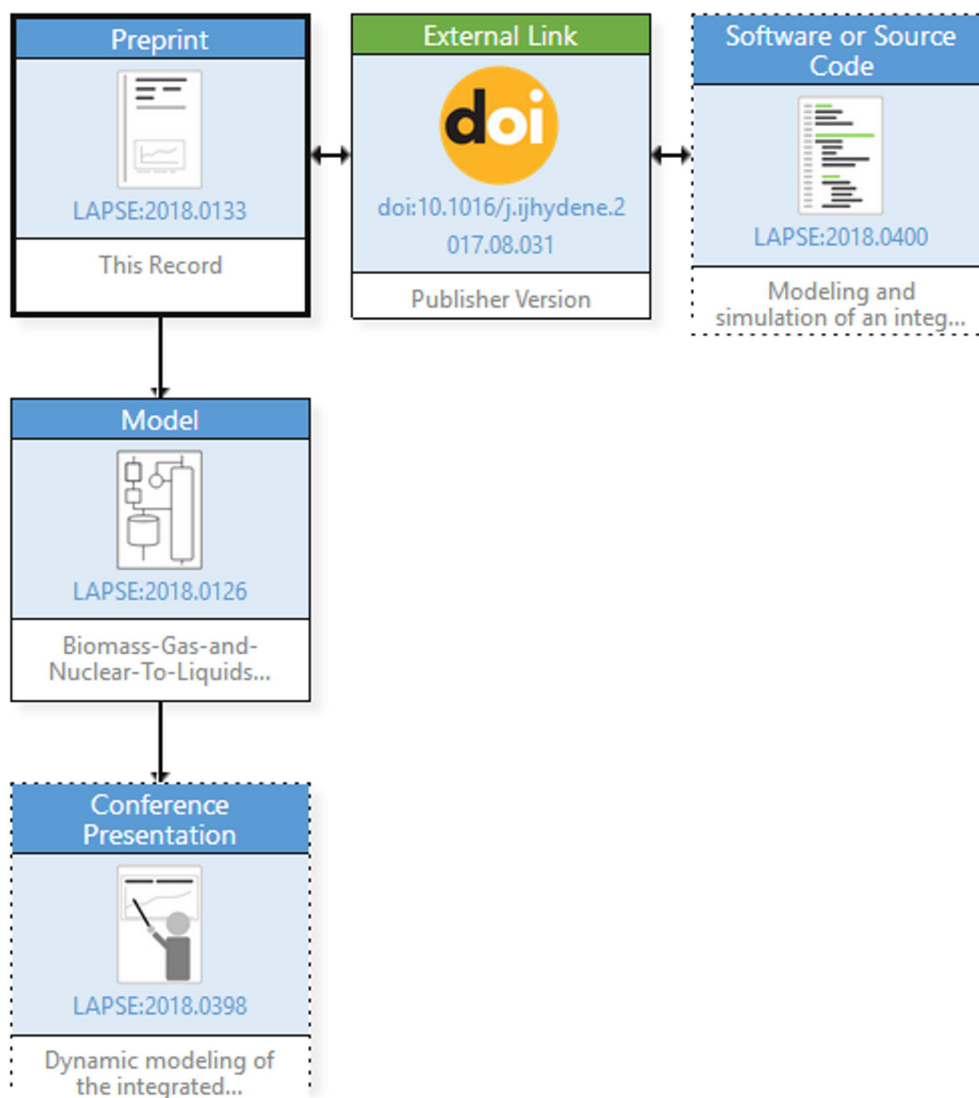
Fig. 4. Record map.

cess publications, open access journals, and major funding organizations that require open sharing of data. LAPSE is only the first step in the movement leading this change; the community must decide the rest.

5. The PSE Technology Tree

To help us prepare for this article, we created a technology tree for process systems engineering. A technology tree maps the progression of research from one technology to another, and how they combine to form new technologies. For example, in order to create a sequential modular process simulator, you must first create an algorithm to solve individual unit operation models, and also create an algorithm to solve sequences of unit operations with recycle using tear streams. Such trees are useful for getting a bird's eye view of both the history of the field and its future directions. However, every researcher might have a different idea about what the tree should look like and how detailed it should be, and the field is always growing. That is why, in the spirit of this conference, we created a Technology Tree Wiki on the website psecommunity.org/pse-technology-tree/. We encourage readers to visit the website and contribute by adding to or changing the structure of the tree. Readers can also create, discuss, or edit ar-

ticles about each individual node, such as providing descriptions, examples, images, videos, or literature citations in each area. In this way, readers can participate in the open creation of an ever-evolving encyclopaedia for our field. An example screen shot is shown in Fig. 5.

One of the key goals of the Technology Tree Wiki is to connect a variety of stakeholders to current research concepts in an accessible way. Readers should be able to find a Technology Tree Wiki article on a topic and then get a good sense not only of the topic itself but where it fits into the larger context of research, thanks to the visual nature of the tree structure. This can help complex research more accessible by breaking down difficult concepts into its more basic components. Moreover, the list of references provide a great starting point for beginning researchers, and as such, readers are encouraged to suggest appropriate citations within the wiki. Moreover, plans are in place to add features that automatically populate the further reading section of each Wiki article from LAPSE submissions so that those reading a Wiki article will see the most up-do-date material on that topic. Similarly, future versions of LAPSE will automatically draw keywords from the Wiki articles that users can select for database indexing and search purposes, and let them link LAPSE records directly to Technology Tree Wiki articles, thus helping them to appear there. In this way, these two

PSE Community.org

The World Community for Chemical Process Systems Engineering Education

HOME   TEXTBOOKS ⌄   EDUCATIONAL MATERIALS ⌄   DISCUSSION BOARDS   CONTRIBUTE
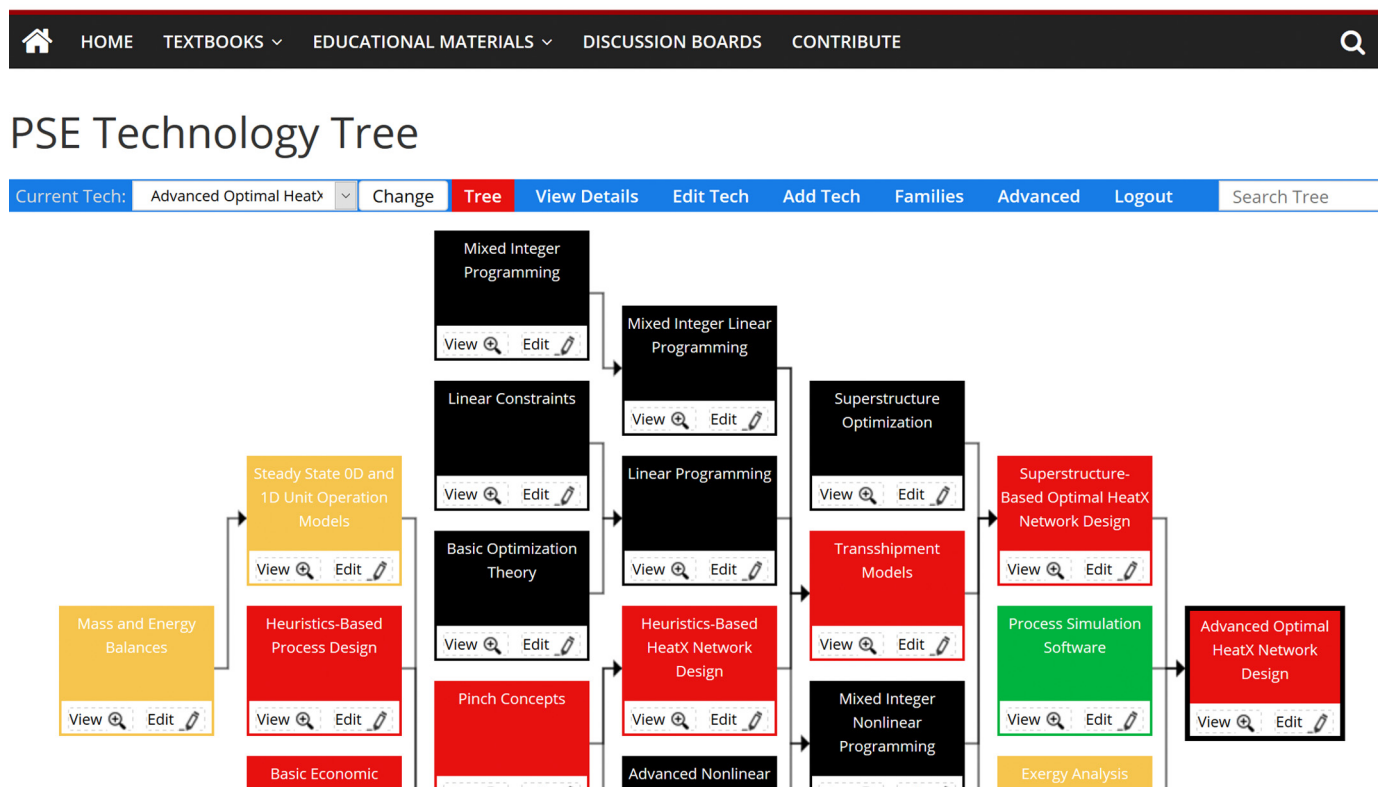
PSE Technology Tree

Fig. 5. A screen capture from the PSE Technology Tree Wiki at PSEcommunity.org.

tools can work together to increase research and educational impacts within the field.

6. Conclusions

From a big picture perspective, the historical progression of the field of process design is perhaps best characterized by an ever-increasing problem scope. Our fundamental understanding behind major chemical unit operations and their thermophysical phenomena has not changed much over the decades. Instead, the *methodology* of process design has expanded to include more and more rigorous mathematical, dynamic, control, planning, scheduling, product design, uncertainty, economics, and environmental factors, although not yet all at once. All of this is made possible by continually improving numerical methods (particularly optimization and modelling) and software tools which make larger and larger problems more tractable.

Based on the extrapolation of this trend, we envision that the future of process design will be largely driven by software that essentially includes all of these areas integrated together in one large global optimization problem. The designer would specify key objectives (perhaps in plain language) that relates to either particular products or merely product properties. Unit operation, process section, or whole-process models would be drawn from open-access databases such as LAPSE. The software would then formulate and solve an optimization problem which automatically synthesizes the design of the dynamic process and its products, together with its dynamic supply chain, plans and schedules, target markets, control systems, and considering all operational details including prod-

uct flexibility and transitions, startup, shutdown, safety, reliability, uncertainty, and disturbance response. Candidate processes would be ranked on metrics that include a mix of environmental, business, and social factors. Data for environmental impacts, markets, supply chains, unit operations, and chemicals would be automatically drawn from massive databases or database-driven models. The process synthesis would be achieved through AI algorithms which draw upon massive models or databases of both human-derived and AI-created processes, heuristics, and best-practices. All of these aspects already exist in one form or another, it is merely the integration of everything together into one mega-problem that remains.

Acknowledgement

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