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REVIEW

Design for environment: a state-of-the-art review

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Abstract Traditional process design concentrates on process simulation and profitability. However, for design for environment one has to extend the simulation framework to include chemical and process synthesis steps and multiple objectives for environmental and societal impacts. This article describes the developments in process design for environmental considerations. Incorporating environmental considerations in the early stages of design like chemical synthesis and process synthesis has larger impact on the design. Therefore, number of approaches and case studies in chemical and process synthesis for environment are presented here. Defining environmental impacts is more difficult than profitability. New models for defining environmental impacts is the focus of some papers important for design for environment. Uncertainties are large in these steps and need to be included in the computational procedures. Further, multiple objectives are involved in process design increasing the complexity of problem.

Keywords Process design · Process synthesis · Computer aided molecular design · Environmental impacts · Sustainability · Green engineering

Introduction

The early methods for computer-aided process design involved models for unit operations, later leading to chemical process simulator technology with the first simulator appearing in the horizon in 1951 and with commercial simulators like ASPEN (Evans et al. 1979) emerging in late 1970s. These commercial simulators are now widely used in chemical industries, national laboratories, and academia for process design and optimization. However, only recently people have started thinking about incorporating green engineering in process design (Diwekar 2003).

Figure 1 shows steps involved in traditional process design. As shown in the figure, process design starts with chemical synthesis where the chemical pathway from reactants to the product is defined at the laboratory scale. Process synthesis translates the chemical synthesis to a chemical process. It involves decisions about process units and connections. Simulation, which is the focus of current systems analysis approaches is the next step, in part, because effective simulation programs and models are available. Unfortunately, simulation is the *last* step in decision-making; it predicts *only* the behavior of a given plant (or strategy) if it is, in fact, constructed (or implemented). Therefore, the emphasis on simulation has only limited potential for maximizing performance and reducing costs. Integrating the *other* steps into computer-aided decision making guided by the green engineering principles could lead to less cost-intensive, environmental friendly plants and strategies, reduce technical, economic, and operational risks, and increase efficiency.

Figure 2 shows the integrated framework developed recently (Diwekar 2003) to include the green engineering principles at all stages. Unlike the traditional process design where engineers are looking for low cost options, environmental considerations include various objectives like the long-term and short-term environmental and other impacts. This new framework includes decisions at all levels starting from the chemical or material selection and the process synthesis stages, to the management and planning stage, linked to the green objectives and goals shown on the top

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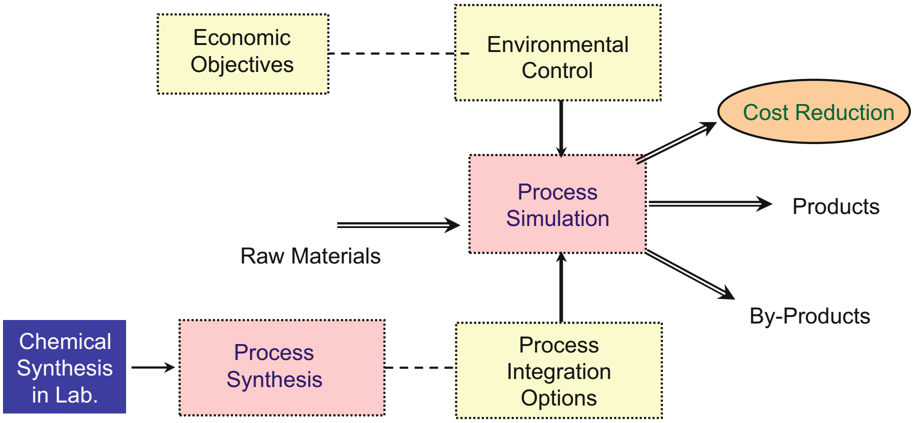

Fig. 1 Traditional process design steps

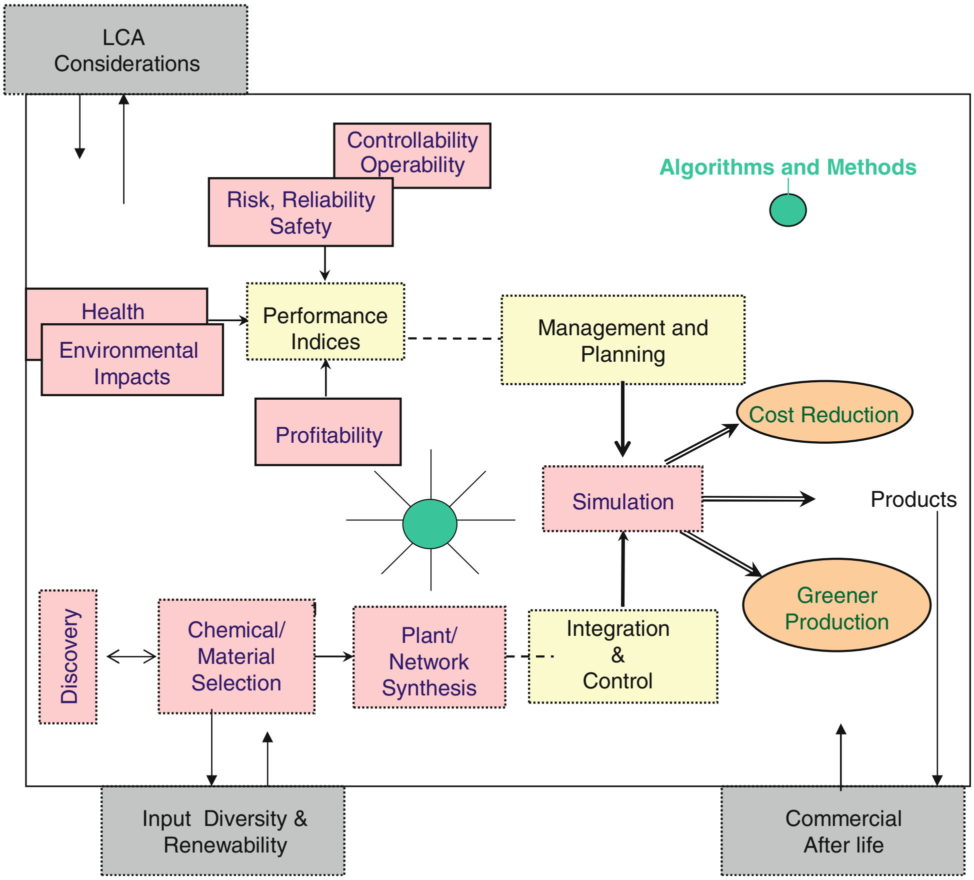

Fig. 2 Integrated framework for green engineering (Diwekar 2003)

left-hand corner of the figure. It is important to start as early as possible in the design process in order to enhance the impact of waste minimization as shown in Fig. 3.

Definition of various objectives is a key component in the design and operation of clean process technologies and is identified to be the most difficult task. The goals in terms of profitability are relatively easy to define, and researchers in academics and industries have used simulators and modeling tools to achieve profitability where environmental considerations are considered as definable constraints. However, the inclusion of "complete ecological considerations" as environmental impact objectives is a formidable task. Thus, multi-objective optimization methods are necessary to handle the conflicting and different objectives involved in the problem of greener by design. Extending the envelop from simulation to chemical synthesis on one end, and management and planning on the other end, and broadening the scope to include multiple objectives other than profitability, increases uncertainties. Further, the decision making then involves discrete decisions related to selection of alternatives, as well as continuous decisions that defines the operations and design of plant.

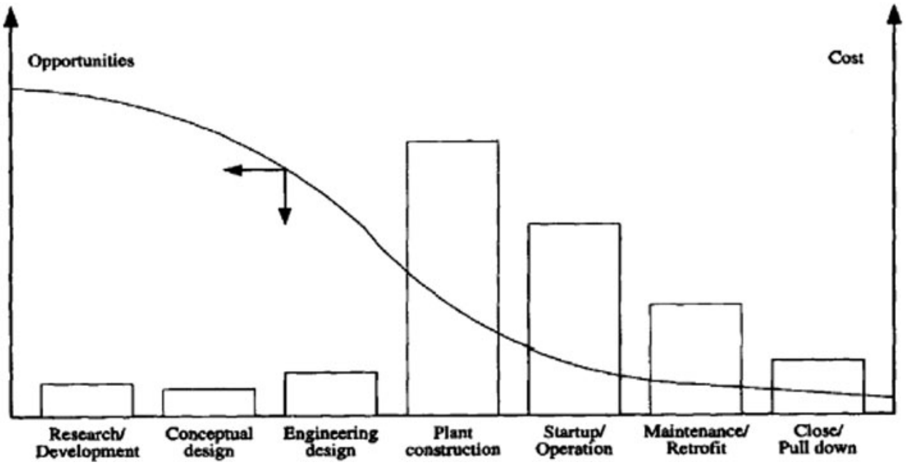

Fig. 3 Opportunities of environmental impact minimization along process life cycle (Yang and Shi 2000)

Research in process design for environment as per steps outlined in the integrated framework shown in Fig. 2 is described in the following sections. Quantification of environmental objectives is presented in "Quantification of environmental aspects indesign framework" section followed by chemical and process synthesis. Process integration is presented in "Process integration" section and process design general information in "Batch process" section. Last section presents Summary.

Quantification of environmental aspects in design framework

As stated earlier, traditionally, the process design methodologies have focussed on improving the design to achieve economic performance indicators such as profitability or net present value. However, greater environmental and safety awareness has motivated the consideration of additional indicators that represent the performance of a design alternative in terms of these additional dimensions. The initial literature used these indicators as constraints, where the goal was to maximize the profitability while achieving certain minimum level of environmental sustainability (Ciric and Huchette 1993; Gupta and Manousiouthakis 1993). However, this approach may eliminate certain design alternatives and consequently lead to a design that is sub-optimal. The recent trend, therefore, is to include the environmental considerations as one of the design objectives (Fu et al. 2000; 2001; Barrato and Diwekar 2005a, b; Chen and Shonnard 2004; Chen et al. 2002; Li et al. 2009). However, since most of the design methodologies are based on rigorous mathematical approach such as simulation and/or optimization, mathematical quantification of these considerations has become necessary. These are generally referred to as performance indicators or metrics.

Sharratt (1999) presents a concise discussion of the environmental performance criteria as relevant to process design and highlighted the importance of considering the whole life cycle of the plant/process/chemical while doing this analysis. The work also presented a guideline that can be followed while defining an indicator. The author particularly stressed that indicators which incorporate the accident potential or emission of fugitive material in a process are particularly difficult and hence often overlooked. Various ideas have been proposed in the literature over the years to formulate the appropriate performance indicators for the design problem. Adu et al. (2008) present a comprehensive comparison of various methods that have been proposed to quantify the environmental, safety, and health hazards in process design. It first conducts a qualitative comparison of the methods followed by a quantitative comparison using case studies. They concluded that no method was conclusively better than the others and the suitability of a particular method depended on the specific application as well as the design stage of the process. One of the most commonly used approach in recent years has been life cycle assessment (LCA) (Fava 1994). The central idea of LCA is to account for all possible upstream and downstream environmental impacts of a raw material, process, or product throughout the life cycle of the project. Azapagic (1999), Burgess and Brennan (2001), and Bakshi (2002) provide an excellent overview of the scope and limitations of life cycle assessment and its application to chemical process selection and design. Selected examples of LCA-based performance indicators being used for process synthesis and design are Shang and Kokossis (2003), Azapagic et al. (2006), Peregrina et al. (2006), Sugiyama et al. (2006), and Papandreou and Shang (2008). The generalized waste reduction (WAR) algorithm has also been proposed as a measure of the environmental performance of a process (Cabezas et al. 1999). It considers nine different impact categories which include four environmental physical potential effects (acidification, greenhouse enhancement, ozone depletion, and photochemical oxidant formation), three human toxicity effects (air, water, and soil), and two ecotoxicity effects (aquatic and terrestrial) (Cabezas et al. 1999). Examples of application of WAR algorithm for process design include Young and Cabezas (1999), Fu et al. (2000; 2001), Barrato and Diwekar (2005a, b), Shonnard and Hiew (2001), Cardona et al. (2004), Halim and Srinivasan (2008) and Ramzan et al. (2008). Zhang et al. (2008) proposed green degree method that uses an approach similar to the WAR algorithm. Each of the nine indicators considered in the WAR algorithm can individually be used as overall indicators, particularly while focussing on very specific processes or products. Maximizing safety or minimizing risk is also a necessary aspect of environmentally benign chemical process design (Mulholland et al. 2001). Process safety assessment tools such as HAZOP (Kletz 1999) and FMEA (CCPS 1992) can be used to identify potential problems. Dow fire and explosion hazard classification (DOW Chemical 1994) and Mond index (King 1998) have been proposed to estimate the fire and explosion hazards in process plants. Edwards and Lawrence (1993) and Heikkilä (1999) have proposed indices for inherently safer process design. In addition to these well-known approaches, other indices that have been proposed include the Environmental Hazard Index (EHI) (Cave and Edwards 1997), Chemical Hazard Evaluation for Management Strategies (Swanson et al. 1997), the EU Risk Ranking Method (Hansen et al. 1999), the material centric method (Palaniappan et al. 2002), and environmental part of EHS method (Koller et al. 2000). Selected applications of these various safety and hazard indices in process design include (Palaniappan et al. 2002, Koller et al. 2000, Heikkilä et al. 1996, Mansfield and Cassidy 1994).

It must be realized that the appropriate environmental indicator will depend on the case being analyzed as well as the design stage. During the early design stage, when extensive data related to various process alternatives is scarce, a data intensive approach is not appropriate. At this stage, the focus is more on eliminating the worst alternatives rather than identifying the best one. As one proceeds through various design stages, namely, product identification, process synthesis, conceptual design, engineering process design, details plant design, the amount of data available increases. Consequently, data intensive performance indicators become more accurate and suitable. The following sections present various design stages necessary to reduce environmental impacts.

Chemical synthesis

Chemical synthesis involves identifying molecules (chemicals) that can result in products that can be manufactured when process is designed. Environmental consideration at this stage can have a great impact on the process and products being greener or not. Therefore, it is imperative to expand the process design framework to include chemical synthesis decisions for greener process results. The Computer-Aided Molecular Design (CAMD) methods are useful in this regard.

CAMD is generally the *reverse* use of the group contribution method that is used to generate molecules having desirable properties. A basic diagram of CAMD is shown in Fig. 4, in which there is a set of groups as a starting point. These groups are uniquely designed to generate all possible molecules by exploring all possible combinations. The properties of each group and/or the interaction parameters between groups can be theoretically calculated, experimentally obtained, or statistically regressed. From this set of groups, solvent molecules can be generated by group combinations. For example, ethanol (CH_3CH_2OH) is generated from the CH_3, CH_2, and OH groups. Constraints from physical and chemical properties, as well as those from regulatory restrictions, may be imposed, and hence the number of combinations can be reduced. Once molecules are generated, the properties of the molecules are predicted based on the properties of their groups in order to determine if they satisfy the specified criteria. This method can generate lists of candidate molecules with reasonable accuracy within moderate time scale.

Group contribution methods like UNIFAC (Fredenslund et al. 1977) are the basis of CAMD methods. Few articles appeared on use of neural network models for property estimation (Bunz et al. 1998; Yamamoto and Tochigi 2008). Recently, people tried to combine molecular simulations and molecular dynamics methods with group

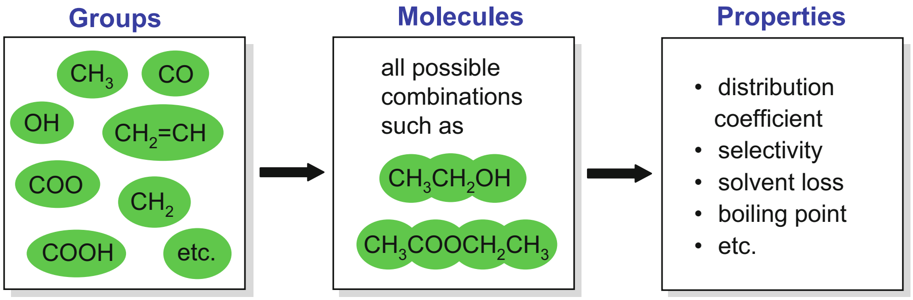

Fig. 4 A basic diagram of CAMD based on group contribution methods (Kim and Diwekar 2002a)

contribution methods (Harper et al. 1999). For property estimation models such as group contribution methods for process and product design, recent review papers by Gani (2004a, b) and O'Connell et al. (2009) provide the perspective, review, and references to various articles including reviews published on this topic of structure property relationship.

CAMD techniques can be classified in terms of their solution algorithm into heuristic numeration (Trevizo et al. 1986; Hostrup et al. 1999; Joback and Stephanopoulos 1989; Li et al. 2002), knowledge-base approaches (Bolis et al. 1991; Gani et al. 1991; Harper and Gani 2000; Yamamoto and Tochigi 2008), molecular property clusters with algebraic equations (Chemmangattuvalappil et al. 2009; Eden et al. 2004; Eljacka and Eden 2008; Vasiliki et al. 2007) and optimization-based methods. Recently, Trevizo et al. (1986) and Adhvaryu et al. (2000) have used multivariate analysis in screening solvents. The heuristic numeration and knowledge-based approaches are based on the formation of all possible molecular structures from a specified set of building groups and the screening of the generated molecules according to molecular design feasibility rules and pre-selected target physical property values. In optimization approaches, reverse problem of finding groups and molecules providing specified properties is formulated as a mixed integer nonlinear programming problem. A number of deterministic optimization methods have been proposed to solve CAMD problems, such as local optimization approaches (Karunanithi et al. 2006; Macchietto et al. 1990; Odele and Macchietto 1993; Pistikopoulos and Stefanis 1998), global optimization approaches like branch and bound (Sinha et al. 1999; Wang and Achenie 2002; Ostrovsky et al. 2002), interval analysis (Achenie and Sinha 2003) and special decomposition method (Karunanithi et al. 2005), hybrid method (Harper et al. 1999), and mixed-integer dynamic optimization (Giovanoglou et al. 2003). As an alternative to local optimization methods, probabilistic methods like genetic algorithms (Venkatasubramanian et al. 1995; Xu and Diwekar 2005, 2006; Cheng and Wang 2008; Kim and Smith 2004), simulated annealing (Kim et al. 2001; Gani 2004; Kim and Diwekar 2002a, b; Kim et al. 2004; Gani et al. 2008), and tabu search (Lin et al. 2005) are adopted to obtain better solutions. CAMD methods have been applied to many areas (Li et al. 2002), such as extraction solvents (Giovanoglou et al. 2003; Marcoulaki and Kokossis 2002; Cheng and Wang 2008), polymer designs (Harper et al. 1999), degreasing solvents (Adhvaryu et al. 2000), blanket wash solvents (Sinha and Achenie 2001; Chemmangattuvalappil et al. 2009), absorption solvents (Eden et al. 2004; Odele and Macchietto 1993; Pistikopoulos and Stefanis 1998), refrigerant design (Churi and Achenie 1995; Duvedi and Achenie 1996), distillation solvents (Kim and Diwekar 2002b; Kim et al. 2004; Xu and Diwekar 2005, 2006; Kim and Smith 2004), reaction solvents (Lin et al. 2005; Folic et al. 2008), catalysts (Lin et al. 2005), value added products (Camarda and Sunderesan 2005), crystallization solvent (Karunanithi et al. 2006), and foaming agents (Yamamoto and Tochigi 2008). Solvent design has attracted significant interest over the last two decades, not only because of the important role of solvents in process operations, but also because of the need to find substitutes for previously used solvents due to environmental, safety, and health regulations. In general, environmental considerations are included in solvent designs as constraints, however, in order to have a holistic approach, environmental considerations need to be part of the objective. Very few researchers (Kim and Diwekar 2002b; Kim et al. 2004; Xu and Diwekar 2006; Gani et al. 2008; Cheng and Wang 2008) have looked at environmental considerations as a multi-objective problem due to the computational intensity of this problem. Further, it has been found that group contribution methods have significant uncertainties in the interaction parameters due to experimental errors and modeling uncertainties. These uncertainties can change the designs significantly. Diwekar and co-workers (Kim and Diwekar 2002a, b; Xu and Diwekar 2005) have considered the inherent uncertainties present in group contribution methods of CAMD. They presented characterization and quantification of uncertainties in Hanson's solubility parameter estimation method used for extraction (Kim et al. 2001) and UNIFAC interaction parameters (Kim and Diwekar 2002a, b; Xu and Diwekar 2005) applied in distillation and used methods for optimization under uncertainty to obtain environmentally benign solvents. Integrating chemical synthesis, i.e. CAMD, with process synthesis and design is the focus of some recent papers (Hostrup et al. 1999; Kim and Diwekar 2002b; Kim et al. 2004; Xu and Diwekar 2005, 2006) particularly addressing environmentally benign solvents and process designs.

Process synthesis

Incorporation of pollution prevention concepts into design and development at initial stages leads to processes that are less cost-intensive and environmentally friendly. Therefore, process synthesis remains an important step in analyzing and designing environmentally benign processes. Since 1978 till recently, several review articles appeared on the topic of process synthesis (Halvacek 1978; Motard 1979, 1983; Nishida et al. 1981; Siirola 1996; O'Young and Natori 1996; Grossmann and Daichendt 1996; Yang and Shi 2000; Alexander et al. 2000; Westerberg 2004; Barnicki and Siirola 2004; Li and Kraslawski 2004; Harmsen 2004). These articles provide the journey of this area through time.

The synthesis approach to green process design is classified into three categories, namely (1) knowledge-based approach, (2) thermodynamic approach, and (3) optimization approach (Chachaudhuri and Diwekar 1998). Process synthesis literature also can be categorized by various synthesis problems addressed in the literatures (Nishida et al. 1981) like reaction path synthesis, reactor network synthesis, separation sequence synthesis, reactor/separation sequence synthesis, heat exchanger network synthesis, and mass exchanger network synthesis (see "Process integration" section for the last two approaches). The literature is rich in heuristic and algorithmic approaches to these problems.

Advances in knowledge-based approaches applied to process synthesis involve methods, in which particular pollution prevention ideas are transferred from one process to another (Slater et al. 1992), and artificial intelligence approaches for developing environmentally friendly chemical processes (Edgar and Huang 1992). Perhaps, the most systematic knowledge-based approach is the hierarchical decision procedure that involves logical sequence of flowsheet evolutions (Douglas 1988). In this procedure, the essential decisions for developing a flowsheet at each level are identified, and if these decisions are altered, then process alternatives are generated. This is usually followed by an economic study of the different alternatives, so that only the viable process options are considered for the next evolutionary stage. The hierarchical approach has also been represented by the "onion model" (Smith 1995), which characterizes the synthesis task as a set of nested decisions pertaining to different operations, as depicted in Fig. 5. As the reaction system is the key component in transforming the raw material into valuable products, it forms the core of the synthesis exercise. The reaction system defines the nature of separation and recycling system, which in turn influences the design of heat exchanger networks. Any excess requirement or deficit related to the heat content of process streams must be handled by heat and cold utilities, affecting the design of utility system. A similar procedure was outlined by Douglas for the synthesis of processes, keeping in view the environmental objective of minimizing waste in process industries (Douglas 1992). The procedure related to process synthesis for waste minimization follows a hierarchical approach, similar to the "onion model," and is summarized in the following paragraphs.

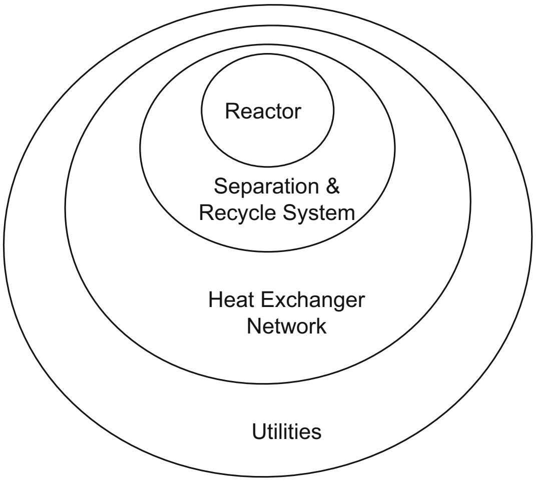

Fig. 5 The onion model adopted from (Smith 1995)

- Level 1: *List input information*. In this level, information regarding the production rate, product value, purity, reaction rates, conditions, raw materials costs, streams, product distribution, catalyst properties, processing constraints, plant site, physical property data, data concerning safety, toxicity, environmental impact, and cost data for the by-products generated (including the "wastes," which have negative economic value) are obtained.
- Level 2: *Define input–output structure of the flowsheet*. The decisions that must be considered at this level pertain to the need to purify the feed streams, whether to recover and recycle some of the reactants, and the necessity of recovering and recycling by-products formed by secondary reversible reactions. In cases where waste minimization problems are caused by the reaction chemistry, it is recommended that alternative pathways for transforming raw materials be investigated.
- Level 3: *Specify the recycle structure of the flowsheet*. The recycling decisions depend on the excess reactant at the reactor inlet, the addition of diluent such as stream to shift the equilibrium or act as a heat carrier, and the need for adding an external solvent to the process. Problems caused by adding diluents and solvents must be eliminated by changing them in favor of a suitable solvent, given environmental objectives of the process.
- Level 4: *Identify the separation systems*. It is desired that the first attempt in the synthesis of separation system involves phase splits. If phase split is not possible, other types of separation systems are also used. For example, vapor recovery systems are used to prevent valuable components from leaving the process with gaseous streams. Liquid recovery systems are used to separate components between phases or to separate liquid mixtures. In this context, distillation is the most preferred from a pollution prevention point of view, because other means, such as the use of extractive agents or spent adsorbents often results in pollution problems. Solid recovery systems, such as filtration, involve cake washing resulting in additional water

treatment facilities. However, it should be remembered that distillation is not a good separation in the point of view of energy consumption.

- Level 5: *Evaluate the alternatives*. This is guided mostly by economic considerations and influenced by environmental objectives. The main drawback is that the evaluation and screening task becomes tedious in the presence of several alternatives.
- Level 6:*Flexibility, control, and safety*. This level involves decisions related to the operability, controllability, and safe operation of the plant.

The hierarchical approach, based primarily on heuristic methods, relies on intuition and engineering judgement for quick selection of alternative process configurations. Although, this is an advantage in the generation of alternatives, the solutions that some heuristics rules predict are poor. Further, heuristic rules may contradict one another and may require assigning arbitrary weights to resolve conflicts.

Thermodynamic approaches to process synthesis are related to process integration and consider waste minimization objectives explicitly. Hence, a separate section is devoted to these approaches based on pinch technology.

The complexities of chemical processes involving environmental implications and the vast majority of promising candidate technologies are inhibiting the screening and selection procedure for the "optimum" process technology. This, coupled with the fact that numerical computations are less expensive now a days, has resulted in the acceptance of optimization approaches for evaluating and screening candidate technologies to identify the best option based on any given criterion. The main idea in this approach is to formulate the synthesis task as an optimization problem. This involves integrating sophisticated optimization techniques into process simulation models and requires an explicit or implicit representation of a specified set of process alternatives from which the optimal solution is derived. This provides a more systematic framework for handling a variety of synthesis problems with single or multiple objectives. Early approaches based on optimization, which were applied to a number of waste minimization problems, depended on mathematical models to develop costs versus emission limit curves (Rossiter 1994). These enabled engineers to understand the effect of fundamental process changes on the costs and emission levels, which were then used to define the least cost-intensive means of achieving a given emission target. A multi-objective optimization process synthesis approach proposed and implemented recently provides a trade-off surface for various objectives and presents a useful tool for decision maker (Dantus and High 1999; Goyal and Diwekar 2001; Johnson and Diwekar 2001; Kim and Diwekar 2002b; Xu and Diwekar 2005).

The optimization approach to process synthesis, by virtue of the advances in the field of computers, has gained much prominence in recent literature related to design for environment (Steffens et al. 1999; Kheawhom and Hira 2002; Dantus and High 1999; Chachaudhuri and Diwekar 1998; Diwekar et al. 1992; Diwekar and Rubin 1993; Halim and Srinivasan 2008; Narayan et al. 1996; Chaudhuri and Diwekar 1999; Dantus and High 1999; Goyal and Diwekar 2001; Linninger and Chakraborty 1999; Kim and Diwekar 2002b; Xu and Diwekar 2005; Kheawhom and Hira 2004; Fresnedo et al. 2007). The approach can be simply stated as follows: Given a set of structural alternatives or options in a process (e.g. a set of environmental control options, a set of heat exchanger network configurations, a set of separation system configurations) which are represented by integer variables, design and operating variables (real continuous variables), an objective and a set of constraints (model equations), the goal is to find the optimal configuration for the process flowsheet and optimal process design. The resulting discrete continuous optimization problem can be solved by mixed integer nonlinear programming (MINLP) algorithms like outer approximation (and variants) (Diwekar et al. 1992; Diwekar and Rubin 1993; Fresnedo et al. 2007), branch and bound (Narayan et al. 1996), or using probabilistic methods like genetic algorithms (Xu and Diwekar 2005, 2006; Kheawhom and Hira 2004), or simulated annealing and (variants) (Chachaudhuri and Diwekar 1998; Goyal and Diwekar 2001; Kim and Diwekar 2002b) procedures. Since synthesis problems considering environmental impacts are fraught with uncertainties, algorithms for synthesis under uncertainties (Chaudhuri and Diwekar 1999; Kheawhom and Hira 2002; Kim and Diwekar 2002c; Xu and Diwekar 2005) and multi-objective process synthesis (Steffens et al. 1999; Kheawhom and Hira 2004; Xu and Diwekar 2006) received greater attention recently. An approach combining heuristics with P-graph approach (optimization based) followed by multi-objective optimization for synthesizing environmentally benign processes has been proposed in the form of expert system by Srinivasan and co-workers (Halim and Srinivasan 2008, 2009).

Process integration

Process design and integration has been a topic of intense research for the last couple of decades. Cano-Ruiz and McRae (1998) give a comprehensive overview of the various aspects of process design which includes, problem framing, generation of alternatives, analysis of the alternatives, evaluation and optimization and sensitivity analysis. While initially the focus was mainly on process synthesis and waste minimization, the importance of process integration and retrofitting as a means to improve environmental performance has increased in recent years. Yang and Shi (2000) review the overall progress in process design in the 1990's and discuss aspects related to process integration.

Process integration is described as "a holistic approach to process design, retrofitting, and operation which emphasizes the unity of the process" (El-Halwagi 1997). This approach often has the environmental dimension that should be acknowledged. The initial focus in process integration was mainly on energy savings, and pinch technology emerged as one of the most widely used process integration tool (Linnhoff and Hindmarsh 1983). Process integration using pinch analysis involves two stages. First, the process under consideration and various streams within the process are analyzed to determine the minimum requirement of energy. This also highlights the potential plant wide energy savings. In the second step, the heat exchange network is synthesized that aims to achieve the theoretically possible energy savings. The problem table algorithm (PTA) was proposed as a means of determining the optimal energy targets followed by the generation of composite curves (CC) (Linnhoff et al. 1982). Salama (2006) has instead proposed a geometry based approach where the composite curves are first constructed followed by the determination of the optimal heat energy targets, heat pinch point location, and grand composite curve (GCC). Liebmann et al. (1998) applied pinch analysis for energy conservation in crude oil distillation, while Fritzson and Berntsson (2006) have applied it reduce energy demand in meat processing plant by almost 30%. Other selected examples of the application of pinch technology in energy conservation are (Sorin and Paris 1997; Briones and Kokossis 1999). Stehlik et al. (1995) argued that in order to achieve better overall design, utilities must be analyzed along with the plant and proposed pinch analysis for heat integration with the inclusion of furnace. In most of these applications, important energy savings have been observed. Looking at it from life cycle assessment perspective, energy saving can be directly correlated to less emissions (based on how the energy is being generated). Therefore, these improvements lead to a more environmentally compliant process design.

The success in the application of pinch analysis for heat integration and saving paved way for its application to mass integration. Mass pinch analysis aims to minimize waste generation and material use by innovative process integration (Gupta and Manousiouthakis 1994). Water has been a focus of many studies since the overall environmental impact can be reduced though water conservation (Alva-Argez et al. 1999; Ku-Pineda and Tan 2006). A state-of-the-art review appeared recently in this area (Chwan and Foo 2009). Kim and Smith (2004) proposed a mixed integer nonlinear programming approach to analyze discontinuous (dynamic) water networks where time is an important dimension. Hul et al. (2007) used a mathematical programming approach for integration of water networks and used particle swarm optimization to solve the mixed integer nonlinear programming problem. A significant amount of progress has also been made in the area of combined heat and mass analysis from the perspective of process integration (mass and heat integration) (El-Halwagi et al. 1995; Leewongtanawit and Kim 2008). Dunn and Bush (2001) proposed the CLEANER (Combined Lower Emission And Networked Energy Recovery) design strategy in which process integration constitutes an important component. They classify the process integration methodologies into energy conservation and waste reduction design methodologies, both of which can include end-of-pipe design or in-plant process design.

From the methodological perspective, process integration techniques include mathematical programming approaches such as mixed integer linear and nonlinear programming. Multi-objective optimization methods can be a valuable tool to study the trade-off between different design objectives. Marechal and Kalitventzeff (1996) combined pinch analysis with mixed integer linear programming while Novak Pintaric and Glavic (2002) and Kralj et al. (2005) used pinch analysis in combination with mixed integer nonlinear programming. Knowledge-based approaches, such as expert systems, rely on a set of predefined rules which are used to screen through the possible design alternatives. Software packages based on this approach include EnvironCAD (Petrides et al. 1994) and CPAS (Shanley 1995).

Batch process

Batch processes constitute an important part of the chemical industry and are quite commonly used in the manufacturing of pharmaceutical products, food products, and speciality chemicals. Batch processes are often carried out in campaigns where a specific chemical is manufactured for a fixed period to time. The same set of equipment is then used to manufacture a different product. Such production schemes are suitable for high value products for which demands might be seasonal. However, this flexibility poses significant challenges for process design and scheduling. Process design is constrained by the existing equipment availability and conditions. Moreover, process dynamics become very important for operability and controllability issues. However, the most critical issue with batch processes is often energy and waste management. Batch processes often generate large quantities of wastes due to the requirements of product separation and equipment cleaning. Batch processes in pharmaceutical industries are especially known to generate large quantities of waste per unit of the finished product (Linninger et al. 1994; Sheldon 1997). Hence, batch process design has been a challenging topic of research within the process systems engineering community.

The literature on systems theory based approaches for batch process planning and scheduling is vast. The focus here is to highlight some of the important contributions that incorporated environmental/ecological factors in batch process design. A significant focus initially was devoted to energy/heat management within the multi-product batch processes. Both sequential as well as simultaneous approaches for this, each with its advantages and limitations, have been proposed. Simultaneous approaches often employ mathematical programming approaches (such as MILP, MINLP formulations) and their variants to determine the optimal schedule. Selected examples of such approaches include Papageorgiou et al. (1994), Lee and Reklaitis (1995), Vaklieva-Bancheva et al. (1996), Pinto et al. (2003), and Majozi (2006). Adonyi et al. (2003) proposed a graph theoretic approach for simultaneously performing process scheduling and heat integration. Sequential approaches often more suited for complex problems where simultaneous consideration of multiple objective was not possible. Grau at al (1996) developed a methodology for production planning and scheduling of multi-product batch chemical processes that considered waste and energy minimization in addition to economic factors. The methodology followed a sequential approach where design alternatives using the economic criteria were modified to address waste minimization and energy saving objectives. Halim and Srinivasan (2009) also proposed a sequential approach which uses a stochastic search-based integer cut procedure to constraint scheduling formulations (master problem). Other examples of the use of a sequential approaches include Vaselenak et al. (1986) and Corominas et al. (1993). Bieler et al. (2003, 2004) instead modeled energy consumption in batch plants using two different approaches (top-down and bottom-up) to identify important energy saving potential that can then be the focus of a rigorous optimization analysis.

The initial focus on heat integration led to a wider focus on other environmental issues in batch process design. Wand and Smith (1995) focused minimized freshwater intake while Foo et al. (2005) worked on the synthesis of water recovery networks. Zhaoling and Xigang (2000) considered raw material selection for batch processes and defined EQW (Effective Quantity of Waste) as the environmental impact assessment criteria. Linninger et al. (1995, 1996) developed the *BatchDesign-Kit* software that enables the determination of various ecological indicators such as chemical toxicity, health/safety hazards, and environmental impacts for a particular process configuration. A rule-based expert system was used to screen materials through the federal, state, and local regulations. Halim and Srinivasan (2008) have proposed a simulation-optimization framework which combines P-graph-based approach, process simulation, and stochastic multi-objective optimization to optimize the economics and environmental footprint. Realff et al. (1996) focused on pipeless batch plants where the layout of the plant is also an additional important factor. Other recent examples of environmentally conscious batch process design include Lee and Malone (2000), Chakraborty and Linninger (2002), Montagna (2003), Halim and Srinivasan (2006), and Carvalho et al. (2009).

Process design: general information and methodological contributions

Process design literature is also replete with a number of new methodological approaches to solve design problems more efficiently where operating conditions and design decisions are decided . Multi-objective optimization has emerged as an important tool to solve many of the design problems. The environmental performance has emerged as an additional dimension to the conventional economic dimension. This results in a trade-off that is often resolved by solving a multi-objective optimization problem. The solution of the multi-objective problem can be obtained using a conventional mathematical programming approach (such as mixed integer linear programming) (Papandreou and Shang 2008; Li et al. 2009). However, the complexity of such problems in addition to the large solution space has motivated the use of various heuristics approaches, and Genetic Algorithm (GA) has emerged as a often employed approach in this field. Some of the important contributions that include methodological contribution are reviewed below.

Seider et al. (2009) have recently provided an interesting perspective on product design. The authors go beyond just design for environment and talk about product design in general. The authors argue that process design is a part of product design since new product design and development often involved technological modifications in the process. They propose the use of innovation maps and Stage-Gate Product Development Process (SGPDP) as tools to carry out effective product development in large organization. Sarigiannis (1996) proposed a three step “design for environment” method for process design which consists of material selection (using LCA and Petri nets), process plant synthesis and optimization (focusing on safety issues), and industry wide synthesis (using concepts from industrial ecology). Carvalho et al. (2008) instead focused on process design from the perspective of process retrofitting and proposed a systematic methodology to analyze design alternatives. The methodology is proposed in the form of an EXCEL-based software called SustainPro. Process safety is an important component of environmentally conscious process design and Pohjola (2003) proposed an object-oriented approach where safety-related properties of a process are included as process attributes. Halim and Srinivasan (2009) proposed an intelligent system framework combining expert system, process simulator, and mathematical optimization for waste minimization analysis. Chen and Shonnard (2004) presented a hierarchical approach to process design using environmental constraints. The basic idea is to use a step-wise approach where the environmental considerations are incorporated at various stages of process design which include process screening, basic process flowsheeting, and detail design task such as equipment sizing. The last step also incorporated multi-objective optimization and uses MINSOOP (Fu and Diwekar 2004) algorithm for problem solution. Fu and Diwekar (2003) focused on the use of multi-objective optimization for NOx emission reduction in wake of the USEPA regulation in 1998 to reduce the ozone depleting NOx by the utilities. The model considered NOx, SOx, and cost minimization using the technology design as the decision variables and subject to the technology design constraints along with the energy and mass balance. MINSOOP along with efficient sampling technology was used as the optimization algorithm and a Pereto surface was generated that can be used by the decision maker based on the desired preferences. Dietz et al. (2005) focused on the design of multi-product multi-purpose batch plants and used a combination of genetic algorithms and discrete even simulation (DES) approach to solve the design problem. The contribution of DES is to incorporate the dynamic aspect of the batch process such as equipment shut-down or start-up. They mentioned that this approach can be used for multi-criteria optimization where you are optimizing the economic as well as ecological indices. Kheawhom and Hira (2002) discussed process design for the environment in the presence of uncertainty. This article proposed a new methodology for process synthesis where the uncertainty is classified as deterministic uncertainty (with known bounds or scenarios) and stochastic uncertainty (described using a probability density function) which is sampled using Hammersley sequence sampling (Kalagnanam and Diwekar 1997), similar to the approach proposed by Diwekar and co-workers. The two most important objectives for the synthesis problem are first identified and the synthesis problem is further classified into design and operational decisions. In the outer layer, design decisions are first optimized using MOP, while the operational decisions are optimized in the second stage in the presence of uncertainty. Limited LCA and Sustainable Process Index (SPI) are used as the possible environmental metric.

Summary

Computer-aided process design area is well served by availability of chemical process simulators to simulate any new or old process. However, design for environment adds complexities in computer-aided design. This article presented the state-of-the literature review of this area. Unlike traditional design, such process design problems involve multiple objectives, such as environmental and societal impacts, and have been a focus of several papers in the literature. Process simulation is the main step in traditional process design. On the other hand, one has to start design at earlier stages of process design in order to reduce environmental impacts, namely, chemical synthesis (or computer-aided molecular design) and process synthesis. Uncertainties associated with such design problems are larger than traditional process design problems. These could be due to the lack of understanding of the environmental fate of various chemicals and products (such as nanomaterials) or due to unknown human impact of various pollutants (such as carcinogenicity which is often measured on animals). Both of these could be static as well as dynamics. Another aspect is the lack of information on the performance of different processes, especially novel processes. These various issues make process design for environment a challenging task. New approaches and algorithms to solve these difficult problems are therefore being continuously sought and are a focus of various research papers in the recent past.

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