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Process synthesis, design and analysis using a process-group contribution method

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ABSTRACT

This paper describes the development and application of a process-group contribution method to model, simulate and synthesize chemical processes. Process flowsheets are generated in the same way as atoms or groups of atoms are combined to form molecules in computer aided molecular design (CAMD) techniques. The fundamental pillars of this framework are the definition and use of functional process-groups (building blocks) representing a wide range of process operations, flowsheet connectivity rules to join the process-groups to generate all the feasible flowsheet alternatives and flowsheet property models like energy consumption, atom efficiency, environmental impact to evaluate the performance of the generated alternatives. In this way, a list of feasible flowsheets are quickly generated, screened and selected for further analysis. Since the flowsheet is synthesized and the operations in the flowsheet designed through predictive models to match a set of design targets, optimal solution of a given synthesis problem is guaranteed.

1. Introduction

Process synthesis can be considered as the cornerstone of the process design activity (Nishida et al., 1981; Douglas, 1985; Barnicki and Siirola, 2004; Westerberg, 2004), it involves identification of the processing route to produce the desired product, investigation of chemical reactions needed, selection and design of the operations involved in the processing route, as well as calculations of utility requirements, the calculations of waste and emissions to the surroundings and many more. In chemicals-based process synthesis, two types of problems exist: in the first type, one seeks to improve an existing process flowsheet (also known as the retrofit problem), while in the second type; one seeks to find a completely new process flowsheet. Due to the fact that process synthesis problems are by nature combinatorial and open ended, a number of different approaches have been proposed. These approaches can be broadly classified into three main classes of methods: methods that employ heuristics or are knowledge based; methods that employ mathematical or optimization techniques; and, hybrid methods that combine different approaches into one method.

1.1. Heuristics or knowledge based methods

The most commonly used methods to solve the process synthesis/design problem are the heuristics based approaches due to their ease of application. These methods rely on a set of rules based on a combination of experience, insights and engineering knowledge (data) to come up with a feasible process alternative for a given synthesis problem. There are numerous examples in the literature of the use of heuristics to solve the synthesis and design problems from the chemical and related industries. Particularly, heuristics dealing with synthesis of separation processes in the chemical industry are fairly well developed. Siirola and Rudd (1971), developed a systematic heuristic approach for the synthesis of multicomponent separation sequences. Seader and Westerberg (1977) developed a method, which combines heuristics with evolutionary methods for synthesizing simple separation sequences. Douglas (1985) proposed a hierarchical heuristic procedure for synthesizing process flowsheets where a set of heuristic rules are applied at different levels to generate the alternatives. In general, knowledge based methods are structured around three models. First, the data model, which includes a structured framework capturing all the available knowledge. Second, the data mining model, it includes the procedures and rules to extract the knowledge from the data model to be applied to the synthesis problem. Third and

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last, the application model, which includes the rules and methods to apply the knowledge extracted through the data mining model to the synthesis problem. While this approach is relatively simple to implement, due to the nature of heuristics and the available knowledge base one can end up with sub-optimal designs. Also, since the heuristic rules are based on observations made on existing processes, the application of heuristic methods requires careful consideration as they may lead to the elimination of novel process flowsheets.

1.2. Mathematical or optimization methods

This approach requires one to define a mathematical superstructure of all the feasible unit operations along with their interconnections and find an optimal flowsheet with respect to a pre-defined objective function such as energy minimization or profit maximization. A lot of studies have been carried out using this approach, and it has been applied in process synthesis and design for chemicals-based processes. Grossmann and Daichendt (1996) have published reviews on suitable optimization techniques for process synthesis. These techniques are easy to apply for homogeneous systems like heat exchanger networks, distillation sequences, and reactor networks, but more difficult to use for heterogeneous systems like generation of total flowsheets. There are two distinct problems that limit the use of mathematical optimization techniques for heterogeneous systems: (1) generation of the superstructure of all possible alternatives; (2) solving the large optimization problem which is inherent in process synthesis. Various numerical solutions methods (Gupta and Ravindran, 1985; Westerlund et al., 1998; Duran and Grossmann, 1986) have been proposed to solve the resulting MINLP problem, but these algorithms are usually limited to moderately sized problems as large number of integer variables and nonlinear equations may prevent not only in finding the optimal solution but even in obtaining a feasible solution.

1.3. Hybrid methods

Since applications of heuristic or knowledge based methods do not necessarily lead to optimal flowsheets, while mathematical techniques are limited by the availability and application range of the model and/or the superstructure, hybrid methods combine different approaches to solve the synthesis problem more effectively. These methods use the physical insights from the knowledge based methods to narrow the search space and decompose the synthesis problem into a collection of related but smaller mathematical problems. This allows for keeping the simple structure of knowledge-based approaches but replace the fixed rules with guidelines based on physical insights generated through analysis of the behavior of the chemicals. Jaksland et al. (1995) developed a hybrid method for the synthesis of separation processes based on thermodynamic insights. This method uses knowledge obtained based on the physical properties of the mixtures involved in the problem. The calculations of the indicators for each mixture provide the user with guidance to find the matching separation task. These indicators are ratios of physical properties, for example, a high difference in relative volatility is an indication that a separation by distillation is a feasible separation method. Similarly Hostrup et al. (2001) presented a framework based on thermodynamic insights and mathematical programming for three-component distillation system synthesis. The approach proposed in this paper can also be classified as a hybrid method for solving process–synthesis problems.

2. Overview of the process-group contribution framework

The process-group concept introduced by d'Anterroches and Gani (2005) applies the principles of the group contribution approach (Marrero and Gani, 2001) used for chemical property estimation to the synthesis and design of chemical and bio chemical processes (Alvarado Morales et al., 2009; Bommareddy and Eden, 2011; Tula et al., 2014). In a group contribution method for estimating pure component/mixture properties of a molecule, the molecular identity is described by means of a set of functional groups of atoms bonded together to form a molecular structure. Once the molecular chemical structure is uniquely represented by the functional groups, the specific properties can be estimated from regressed contributions of the functional groups representing the molecule. Having the groups, their contributions and their interactions together with governing rules to combine the groups into a molecule, allows us to synthesize molecules and/or mixtures. This is known as CAMD, computer aided molecular design. Let us now imagine that each group used to represent a fraction of a molecule could also be used to represent a chemical process operation or a set of operations in a chemical process flowsheet. A functional process-group would represent either a unit operation (such as a reactor, a distillation column, or a flash), or a set of unit operations (such as, two distillation columns in extractive distillation, or pressure swing distillation). The bonds among the process-groups represent the streams connecting the unit operations, similar to the bonds combining (molecular) functional groups. In the same way as CAMD method (Harper and Gani, 2000) applies connectivity rules to combine the molecular functional groups to form feasible molecular structures, functional process-groups would have connectivity rules to combine process-groups to form structurally feasible process alternatives. Finally with flowsheet property model and corresponding process-group contributions it would be possible to predict various flowsheet properties which can be used as performance indicators for screening of alternatives. For example, in Fig. 1, a simple process flowsheet composed of a reactor, followed by a flash column, followed by distillation and membrane separation process, could be represented with process-groups.

Consider the process flowsheet in Fig. 1. The feed streams to the reactor can be represented by two process-groups; one inlet process-group (iA) for reactant A, and an inlet process-group (iB) for reactant B. Similarly end products are represented by two outlet process-groups: (oC) and (oD). The reactor process-group (rAB/ABCD) representing the reactor has one inlet and one outlet. The process-groups representing a flash (fA/BCD) and a distillation (dCD/B) operation have one inlet and two outlets. Finally, the membrane separator is represented by a membrane process-group (mC/D). From the list of process-groups available a feasible flowsheet structure can be created as shown in Fig. 1. As in group contribution based molecular property prediction (where the same molecular groups may be used to represent many molecules), same process-groups with different chemical species can also be used to represent different tasks in the flowsheet as long as the property of the task matches. This makes the process-groups property dependent but not chemical species dependent. Therefore, the use of the same process-groups to represent different chemical species having similar properties is also valid in the case of process flowsheets. Note, however, that the inlet and outlet streams (bonds) of process-groups must maintain the list of components present in them and that the path of a component through a process-group establishes the flowsheet structure. That is, process-groups (A/BC) and (B/C) can be connected to form [−(A/BC) − (B/C)−] without knowing the identities of the components A, B, and C. The identities of the chemicals (components) are only needed when the properties of the flowsheet need to be calculated.