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Integration of modular process simulators under the Generalized Disjunctive Programming framework for the structural flowsheet optimization

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ABSTRACT

The optimization of chemical processes where the flowsheet topology is not kept fixed is a challenging discrete-continuous optimization problem. Usually, this task has been performed through equation based models. This approach presents several problems, as tedious and complicated component properties estimation or the handling of huge problems (with thousands of equations and variables). We propose a GDP approach as an alternative to the MINLP models coupled with a flowsheet program. The novelty of this approach relies on using a commercial modular process simulator where the superstructure is drawn directly on the graphical use interface of the simulator. This methodology takes advantage of modular process simulators (specially tailored numerical methods, reliability, and robustness) and the flexibility of the GDP formulation for the modeling and solution. The optimization tool proposed is successfully applied to the synthesis of a methanol plant where different alternatives are available for the streams, equipment and process conditions.

1. Introduction

One common approach for the optimization of real chemical process handles continuous process parameters (temperatures, pressures, flowrates, compositions, etc.) as the unique optimization variables while the flowsheet topology is kept fixed. A popular tool to perform this task is the process simulators based on the modular architecture, which are perfectly suited for simulation problems but loses part of its attractiveness for optimization or synthesis problems. In addition, chemical process synthesis also demands to make decisions related to process topology, which implies the inclusion of integer variables as free variables in the model, leading to a Mixed-Integer Nonlinear Programming (MINLP) problem (Biegler et al., 1997; Grossmann, 2002). This fact presents both opportunities and challenges for researchers to develop new tools that facilitate the synthesis of chemical plants to chemical engineers.

The Generalized Disjunctive Programming (GDP) modeling framework introduced by Raman and Grossmann (1994) has brought to Process System Engineering (PSE) community the powerful framework of the disjunctive programming, which was originally developed by Balas (1979, 1998) as an alternative representation of mixed-integer programming problems. GDP allows to model chemical plant synthesis problems through the use of higher level of logic constructs (Hooker & Osorio, 1999; Raman & Grossmann, 1994) that make the formulation step more intuitive and systematic, retaining in the model the underlying logical structure of the problem. GDP represents problems in terms of Boolean and continuous variables, allowing the representation of constraints as algebraic equations, disjunctions and logic propositions (Beaumont, 1990). The development of GDP in the chemical engineering community has led to the development of customized algorithms that exploit this alternative modeling framework. In particular, Turkay and Grossmann (1996) extended the outer approximation (OA) algorithm (Duran & Grossmann, 1986) for MINLPs into a logical-equivalent algorithm. Later, Lee and Grossmann (2000) developed a disjunctive branch and bound.

GDP techniques have been successfully incorporated to many types of PSE optimization problems such as process flowsheet synthesis, design of distillation columns, scheduling and design of batch processes. In 1996, Turkay and Grossmann (1998)Turkay and Grossmann published a paper in which they proposed a GDP algorithm for structural flowsheet optimization problem and tested on several examples, including the synthesis of a vinyl chloride monomer process consisting of 32 units. Process synthesis with heat integration was also solved using disjunctions and logic

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propositions by Grossmann et al. (1998). One year later, Caballero and Grossmann (1999) reported an aggregated model for the synthesis of heat-integrated distillation columns modeled as a generalized disjunctive program. Later, a disjunctive programming model was also applied to the synthesis of distillation column sequences (Yeomans & Grossmann, 2000). In all these works, the problem is entirely described on explicit equations by a general modeling language system, like GAMS (Rosenthal, 2013), and usually relies on simplified models (i.e., shortcut or aggregated methods) for the unit operations in the flowsheet and for the prediction of the physical properties of the components (e.g., for the vapor-liquid equilibrium). The first feature of this approach leads to difficulties, when modeling the problem, in the initialization step, which may converted into a daunting task. On the other hand, the use of simplified models for the unit operations could be not accurate enough to capture key aspects of a real chemical process plant. Moreover, using simplified physical property models can predict inaccurate thermodynamic properties, leading to misleading results.

The disadvantages listed in the last paragraph can be overcome by incorporating process simulators to the synthesis problem. Flowsheeting software provides realistic simulations and hence an optimal solution closer to the real implementation as they offer tailored numerical techniques developed for converging the different units and provides an extensive component database and reliable physical property methods. The usage of chemical process simulators as an implicit model for solving synthesis problems through a MINLP approach is not new. Harsh et al. (1989) developed an interface with a MINLP and FLOWTRAN, for the retrofit of an ammonia process. Diwekar et al. (1992) proposed a MINLP synthesizer using Aspen Plus. Díaz and Bandoni (1996) used a MINLP formulation with an existing ad-hoc process simulator for the optimization of a real ethylene plant. Caballero et al. (2005) proposed a superstructure-based optimization algorithm for the rigorous design of distillation columns that combines a process simulator (Aspen HYSYS) with explicit equations. Latter Brunet et al. (2012) used the same algorithm for the optimization of an ammonia-water absorption cooling cycle implemented in Aspen Plus. Flowsheet process optimization with heat integration has also been performed using an hybrid simulation optimization approach, in which the process is solved by a commercial process simulator (Aspen HYSYS), and the heat integration model is in equation form (Navarro-Amorós et al., 2013). All these works are based on the augmented penalty/equality relaxation outer-approximation algorithm (Viswanathan & Grossmann, 1990). Other process simulators (SuperPro) has also been coupled with a multi-objective Matlab optimizer (Taras & Woinaroschy, 2012).

Another approach for the synthesis problem combines process simulators with metaheuristic algorithms. Although metaheuristic algorithms are not able to guarantee the optimality of the solutions found, they can find solutions for some real-world problems that exhibit high levels of complexity (Gendreau et al., 2010). Perhaps the most serious disadvantages of metaheuristic algorithms are that the number of function evaluations to converge could be large, and as well as they exhibit poor performance in highly constrained systems. A considerable amount of literature supports the integration of a process simulator with an external optimizer based on metaheuristic algorithms. Gross and Roosen (1998) demonstrated the suitability of a genetic algorithm coupled with the process simulator Aspen Plus to optimize arbitrary flowsheets. Leboreiro and Acevedo (2004) also succeeded in problems where deterministic mathematical algorithms had failed, using an optimization framework for the synthesis of complex distillation sequences based on a modified GA coupled with Aspen Plus. The same combination of process simulator and metaheuristic algorithm is adopted by Vazquez–Castillo et al. (2009) to address the optimization of five distillation sequences. Subsequent works used a multiobjective GA (Gutiérrez-Antonio & Briones-Ramírez, 2009) for the optimization of thermally coupled distillation systems (Bravo-Bravo et al., 2010; Cortez-Gonzalez et al., 2012; Gutérrez-Antonio et al., 2011), and for the retrofit of a subcritical pulverized coal power plant with an MEA-based carbon capture and CO_2 compression system (Eslick & Miller, 2011). Finally, Odjo et al. (2011) also presented a general framework for the synthesis of chemical processes using a hybrid approach with Hysys and genetic algorithms.

In this paper we present a new modeling framework for dealing with superstructure-based synthesis problems that exploits the synergistic combination of commercial process simulators with GDP formulation and their corresponding logic-based solution algorithms. As far as these authors know, it has not been reported a simulation-optimization tool for solving the synthesis of chemical plants whose superstructure is drawn directly on the process simulator graphical user interface (GUI). We achieve this aim by developing a GDP modeling system that interfaces with a process simulator (Aspen Hysys) at the NLP step to optimize the structure and parameters of a methanol plant based on a superstructure which involves alternative equipment, process conditions and stream configurations. Our methodology allows easily including soft constraints and logical relationships among alternatives, which ensure feasible solutions. The proposed tool uses the logic based Outer Approximation algorithm and hence it is not required to reformulate the problem as an MINLP.

The remainder of this article is organized as follows. The problem statement is first formally expressed. Then the methodology is introduced. In this section, the logic based outer approximation algorithm, integration of the process simulator in the algorithm and the connection with the external optimization solver are described. The proposed simulation-optimization framework is illustrated through a case study based on a methanol plant in the next section, where the superstructure and the disjunctions are presented. In this section, the results are also briefly described. Finally, we draw the conclusions from this work.

2. Problem statement

Given a superstructure for the synthesis of chemical process plant, with some specifications fixed, determine the optimal process flowsheet that leads to the maximum value of an economic indicator. The solution must include both topological and operational (temperatures, pressures, flow rates) information.

3. Methodology

We have developed a modeling system with the following characteristics:

1. The complete modeling system is developed in Matlab (MATLAB, 2006).
2. Indexing capacities for both algebraic equations and implicit models.
3. Use of Boolean variables, disjunctions and logic propositions. Allowing the direct formulation of the problem as a disjunctive problem without MINLP reformulation.
4. Interfaced with different commercial solvers for NLP, LP, MILP models through Matlab-Tomlab (Holmström et al., 2010), and with homemade implementations of the logic based Outer Approximation algorithm (Turkay & Grossmann, 1996).
5. Communication with process simulators and other third party models, except those developed in Matlab, is done by the Windows COM capabilities.