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Process simulator-based optimization of biorefinery downstream processes under the Generalized Disjunctive Programming framework

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ABSTRACT

Downstream processing of biofuels and bio-based chemicals represents a challenging problem for process synthesis and optimization, due to the intrinsic nonideal thermodynamics of the liquid mixtures derived from the (bio) chemical conversion of biomass. In this work, we propose a new interface between the process simulator PRO/II (SimSci, Schneider-Electric) and the optimization environment of GAMS for the structural and parameter optimization of this type of flowsheets with rigorous and detailed models. The optimization problem is formulated within the Generalized Disjunctive Programming (GDP) framework and the solution of the reformulated MINLP problem is approached with a decomposition strategy based on the Outer-Approximation algorithm, where NLP subproblems are solved with the derivative free optimizer belonging to the BzzMath library, and MILP master problems are solved with CPLEX/GAMS. Several validation examples are proposed spanning from the economic optimization of two different distillation columns, the dewatering task of diluted bio-mixtures, up to the distillation sequencing with simultaneous mixed-integer design of each distillation column for a quaternary mixture in the presence of azeotropes.

1. Introduction

The renewed interest in the field of distillation has been recently promoted by the consistent research on biomass conversion technologies to biofuels and bio-based chemicals. These technologies are based on (bio) chemical reactors that produce highly diluted aqueous solutions. The downstream processing of those mixtures usually involves distillation, leading to high operating costs due to the high heat of vaporization of water (G. Q. Chen, 2009; Xiu & Zeng, 2008). For this reason, attempts to optimize and thermally integrate the purification step (Ahmetovic et al., 2010; Dias et al., 2009; Karuppiah et al., 2008) result in a relevant lowering of the production costs that reduces the economic gap with respect to cheaper fossil-based products (Hermann & Patel, 2007; Sauer et al., 2008). In addition, the optimization of this type of downstream processes, as opposed to hydrocarbon distillation, involves highly nonideal liquid mixtures that demand rigorous thermodynamic models.

In this context, process simulators offer a reliable and rigorous modeling environment that rely on extensive thermodynamic properties databanks and tailored distillation algorithms, in contrast with equation-oriented GDP/MINLP optimization tools that are usually based on shortcut models for the unit operations and for the estimation of physical and thermodynamic properties (Navarro-Amoros et al., 2013). Unfortunately, it has been demonstrated that the optimization tools available within commercial simulation packages are not as effective and flexible as it would be required (Biegler, 1985) due to the high nonlinearity of the equation systems, and to the impossibility to optimize structural (integer) decision variables. This was the motivation for several authors to develop ad-hoc interfaces for the process simulator-based optimization with MINLP optimization algorithms. Two main strategies have been proposed; the one based on the augmented penalty/equality relaxation outer-approximation (AP/ER/OA) deterministic algorithm (Viswanathan & Grossmann, 1990), and the ones based on metaheuristic methods, such as the evolutionary algorithms (Gross & Roosen, 1998).

Starting from the deterministic approach, Harsh and co-workers developed an MINLP algorithm for the retrofit of chemical plants with fixed topology based on the FLOWTRAN process simulator, and they applied it to the ammonia synthesis process (Harsh et al., 1989). Other authors (Diaz & Bandoni, 1996) derived an MINLP approach to optimize the structure and the operating parameters of a real ethylene plant in operation, interfacing a specific simulation code. Caballero et al. (Caballero et al., 2005) proposed

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an optimization algorithm for the rigorous design of single distillation columns using Aspen HYSYS and Brunet et al. (Brunet et al., 2012) applied the same methodology to assist decision makers in the design of environmentally conscious ammonia–water absorption machines for cooling and refrigeration. Very recently, Navarro-Amoros et al. (Navarro-Amoros et al., 2014) proposed a new algorithm for the structural optimization of process superstructures within the Generalized Disjunctive Programming (GDP) framework. Finally, Garcia et al. (Garcia et al., 2014) proposed a hybrid simulation-multiobjective optimization approach that optimizes the production cost and minimizes the associated environmental impacts of isobutane alkylation. The simultaneous process optimization and heat integration approach has been also addressed by coupling process simulators with external equation systems (Y. Chen et al., 2015; Navarro-Amoros et al., 2013).

On the other hand, several authors have proposed optimization algorithms based on evolutionary methods in order to overcome some difficulties that arise from the use of deterministic nonlinear programming solvers with real-world complex problems. For instance, Gross and Roosen (Gross & Roosen, 1998) addressed the simultaneous structural and parameter optimization in process synthesis coupling Aspen Plus with evolutionary methods. Similarly, an optimization framework is proposed (Leboreiro & Acevedo, 2004) for the synthesis and design of complex distillation sequences, based on a modified genetic algorithm coupled with a sequential process simulator, succeeding in problems where deterministic mathematical algorithms had failed. Vazquez-Castillo et al. (Vazquez-Castillo et al., 2009) addressed the optimization of intensified distillation systems for quaternary distillations with a multiobjective genetic algorithm coupled to the Aspen Plus process simulator. Subsequently, Gutierrez-Antonio and Briones-Ramirez (Gutierrez-Antonio & Briones-Ramirez, 2009) implemented a multiobjective genetic algorithm coupled with Aspen Plus to obtain the Pareto front of Petlyuk sequences. Bravo-Bravo and co-workers (Bravo-Bravo et al., 2010) proposed a novel extractive dividing wall distillation column, which has been designed using a constrained stochastic multiobjective optimization technique, based on the use of GA algorithms. Finally, Eslick and Miller (Eslick & Miller, 2011) developed a modular framework for multi-objective analysis aimed at minimizing freshwater consumption and levelized cost of electricity for the retrofit of a hypothetical 550 MW subcritical pulverized coal power plant with an MEA-based carbon capture and compression system.

In this work, a new interface between the process simulator PRO/II (SimSci, Schneider-Electric) and GAMS is proposed for the structural and parameter optimization of downstream processes based on the OA algorithm and on the use of a Derivative Free Optimizer (DFO). The optimization tool is applied to several case studies, including the distillation sequencing with simultaneous mixed-integer optimal design of each distillation column for a quaternary mixture in presence of azeotropes. The paper is structured as follows. Section 2 defines the problem statement, including the main modeling assumptions and the required inputs for the superstructure optimization. Then, the process superstructure (Section 3) and the modeling framework (Section 4) are described. Section 5 addresses the optimization algorithm, while Section 6 reports the solution strategy and discusses implementation issues. Finally, Section 7 provides a selection of application examples in the field of bio-based chemicals downstream processing.

2. Problem statement

The aim of this work is to propose a new algorithm for the topology optimization of complex process superstructures based on rigorous thermodynamic models, with special emphasis on distillation downstream processes in the biorefining area. Specifically, the distillation sequencing problem with simultaneous design of number of trays and feed tray location is addressed. Both continuous (e.g. split ratio, reflux ratio, pressure) and integer (e.g. number of trays, feed trays, equipment existence) decision variables are optimized under the Generalized Disjunctive Programming (GDP) framework (Grossmann & Trespalacios, 2013), using the process modeling environment of SimSci PRO/II, and the optimization environment of GAMS.

The process modeling is based on the assumptions of the process simulator. Particularly, the most representative equipment is the distillation column, which is described as a cascade of countercurrent vapor–liquid phase equilibrium stages, with a constant pressure drop per stage, a constant High Equivalent to a Theoretical Plate (HETP) for structured packing internals, and a kettle-type reboiler.

The optimization algorithm basically requires a superstructure, the propositional logic to define the topology of the superstructure, selected flowsheets implemented in PRO/II, a set of bounded continuous and integer decision variables, nonlinear (potentially implicit) constraints (e.g. purity and safety constraints), and an economic objective function.

3. Process superstructure

The optimization procedure starts from the definition of the process superstructure. The most general superstructure that can be handled by this algorithm is based on the interconnection of permanent units with elementary conditional unit and trays modules. While permanent units are present in each possible optimal flowsheet originated from the superstructure, the elementary conditional unit and trays modules are introduced in the superstructure to describe the conditional units (or conditional sections with more than one unit) that are not necessarily present in the final optimized flowsheet. Conditional trays are introduced within the conditional unit and trays module for the rectification and stripping sections of the distillation columns potentially present (Fig. 1). The GDP conditional tray representation is adopted to define feed stage and number of stages of the distillation column (Barttfield et al., 2004).

It is worth to note that the superstructure is never completely solved as a unique process simulator flowsheet. Rather the model could be depicted as a collection of different possible black-box simulations, which are defined by disjunctions, in contrast with fully equation-oriented models. For this reason, only permanent units and selected conditional units are solved at each call of the process simulator. In this way, no splitters are required for conditional units, and zero-flow units are avoided.

A relevant case of this kind of superstructure arise from the solution of distillation sequencing problems. At this level, it is possible to represent the sequencing with either a State Task Network (STN) or a State Equipment Network (SEN) (Yeomans & Grossmann, 1999). Fig. 2 reports the two different superstructures for the distillation of a ternary mixture. It is possible to highlight that the SEN requires a smaller number of columns but it introduces recycles. Nevertheless, since the modeling is accomplished by the process simulator with a logic-based definition of the input file that considers only selected units, it does not matter if either STN or SEN superstructure is adopted.

4. Modeling

The detailed modeling is achieved with a process simulator (SimSci PRO/II) taking advantage of thermodynamic databanks