**Process Superstructure Optimization through Discrete Steepest Descent Optimization and Applications in Process Intensification**

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**ABSTRACT**

The optimal design of processes is a challenge faced by the Process Systems Engineering (PSE) community. The efficiency, economical, and environmental goals that chemical processes need to satisfy require a systematic procedure to find the optimal design. In particular, recent developments from Process Intensification (PI) techniques have shown to be promising alternatives to traditional processes, where novel ways of integrating and interconnecting units achieve superior processes in terms of the goals or objectives mentioned above (Sitter, Chen, and Grossmann 2019). Different alternatives of process flowsheets can be represented as a process superstructure, where the units that can be potentially included and interconnections are included (Yeomans and Grossmann 1999). This superstructure allows for the equations of the units and interconnections to be included as constraints in a mathematical optimization problem. This optimization problem can be tackled using tools from Mathematical Programming. Given that the constraints describing the units usually involve nonlinear inequalities and can be in terms of both continuous (e.g. flowrates or temepratures) and discrete variables (e.g. choice of equipments, location of interconnections) the mathematical models are usually posed a Mixed-Integer Nonlinear Programs. The solution of these optimization problems is challenging given both their combinatorial and nonconvex nature(Grossmann and Trespalacios 2013).

In order to tackle the modeling and solution challenges of the MINLP problems, the Generalized Disjunctive Programming (GDP) framework has been proposed. In GDP, the modeling capabilities of traditional mathematical programming is extended by the introduction of Boolean variables involved in propositions and disjucntions (Grossmann and Trespalacios 2013). Besides offering a more intuitive modeling paradigm of discrete problems through disjunctions, a GDP model can be used to inform computational solution tools, *solvers*, of the underlying structure of the original problem allowing for performance improvements when optimizing these problems. The GDP framewrok has been particularly successful in addressinng problems derived from process superstructure optimization (Chen and Grossmann 2017).

The tailored solution methods for GDP are usually based on generalizing algorithms for MINLP, where the optimization problems are decomposed in a way where the discrete variables are fixed and allow to solve the problem only in terms of the continuous variables. Different methods are used to select the combination of these discrete variables, including branching across the different values the discrete variables can take (i.e. Branch-and-Bound) or solving a linear approximation of the original problem which takes the form of a Mixed-Integer Linear Program (MILP) (Kronqvist et al. 2019). For the GDP algorithms, contrary to the case of MINLP solution methods, these Nonlinear Programming (NLP) subproblems only include the constraints that concern the logical variable combinations. Among these tailored algorithms we encounter the Logic-based Branch-and-Bound (LBB) and the Logic-based Outer-Approximation (LOA) (Chen et al. 2018). These approaches avoid evaluating numerically challenging nonlinear equations when certain variables are irrelevant (i.e. “zero-flow” issues) and allow for a more efficient exploration of the combination of discrete/logical variables.

Here we present an algorithm for the solution of discrete nonlinear problems arising from process superstructure problems. Our Discrete-Steepest Descent Algorithm (D-SDA) (Liñán et al. 2020a), based on the theory of discrete convex analysis(Murota 1998), allows us to explore the combinatorial space of the discrete variables arising from the process superstructure problems efficiently. The D-SDA relies on a reformulation of the original discrete problem, usually in terms of binary or Boolean variables, into a problem of integer choices that we name *external variables*. The external variables, which are no longer representable in terms of the original problem constraints, provide a succint representation of the interconnection locations. The exploration of the discrete neighborhood of the external variables provides us with an efficient approch to choose which combination of the discrete choices should be considered to solve the NLP subproblems. The D-SDA uses as termination criterion the *integrally local* optimality, allowing it to efficiently solve problems in process superstructure optimization. In (Liñán et al. 2020a) we comapre the given algorithm with traditional MINLP solution methods, highlighting its performance superiority in terms of computational time and solution quality.

Having D-SDA as an efficient tool to solve process superstructure optimization problems, we use it to address the discrete optimization of a PI application involving distillation and chemical reaction. We tackle the production of Ethyl tert-butyl ether (ETBE) from iso-butene and ethanol through the optimal design of a catalytic distillation column (Bernal et al. 2018). The optimal design required us determining the total number of stages in the column and the position of both feeds and catalyst for the chemical reaction while satisfying operating constraints and maximizing an economic objective (Liñán et al. 2020b). Our method proved to be more efficient than commercial MINLP solvers to address this problem. Furthermore, by considering multi-scale phenomena in the distillation modeling, we are able to implement a rate-based model for the mass and energy transfer within the column and succesfully solve this large-scale and nonconvex discrete nonlinear problem. We present D-SDA, a disjunctive algorithm specially designed for process superstructure optimization based on discrete convex analysis that we have proved empirically to be more efficient that MINLP solution methods and that has allowed us to tackle challenging problems addressing Process Intensification.

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