Engineering 3 (2017) 202–213

Contents lists available at ScienceDirect

Engineering

journal homepage: www.elsevier.com/locate/eng

Research
Smart Process Manufacturing—Article

Nonlinear Model-Based Process Operation under Uncertainty Using Exact Parametric Programming

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ARTICLE INFO

Article history:
Received 30 November 2016
Revised 8 February 2017
Accepted 28 February 2017
Available online 24 March 2017

Keywords:
Parametric programming
Uncertainty
Process synthesis
Mixed-integer nonlinear programming
Symbolic manipulation

ABSTRACT

In the present work, two new, (multi-)parametric programming (mp-P)-inspired algorithms for the solution of mixed-integer nonlinear programming (MINLP) problems are developed, with their main focus being on process synthesis problems. The algorithms are developed for the special case in which the nonlinearities arise because of logarithmic terms, with the first one being developed for the deterministic case, and the second for the parametric case (p-MINLP). The key idea is to formulate and solve the square system of the first-order Karush-Kuhn-Tucker (KKT) conditions in an analytical way, by treating the binary variables and/or uncertain parameters as symbolic parameters. To this effect, symbolic manipulation and solution techniques are employed. In order to demonstrate the applicability and validity of the proposed algorithms, two process synthesis case studies are examined. The corresponding solutions are then validated using state-of-the-art numerical MINLP solvers. For p-MINLP, the solution is given by an optimal solution as an explicit function of the uncertain parameters.

1. Introduction

The design and operation of process plants are subject to a number of uncertain parameters, such as fluctuating production outputs, ever-changing market prices and demands, and so on. A weakening product demand, catalyst deactivation, or financial woes for the corporation are but a few of the multitude of potential causes for optimizing the process. In order to ensure that the optimal process has been designed, it is imperative to certify that the proposed design operates both economically and safely, should physical or socioeconomic changes occur. Process synthesis [1] is a key aspect of plant design, having a significant financial impact on a firm. This has subsequently inspired substantial research in the field, in order to devise methods that will accurately design not only the optimal route, but also the most robust route. Furthermore, due to the computational complexity of the problem, it is essential that the formulated algorithms are efficient in order to minimize the computational cost. In general, the process synthesis problem for a chemical plant can be classified as an integrated system of the following major components: ① heat-exchanger network (HEN) synthesis, ② reactor path synthesis, and ③ separation systems synthesis. Reactor path synthesis is conducted to determine the optimal reactor configuration for a desired product. Within this problem, a number of factors ranging from the thermodynamic boundaries of the system to the reaction path are considered. There are three main techniques used for the optimization of reactor networks: the superstructure approach, the geometrical approach, and the combined targeting approach [2]. The superstructure approach requires a simultaneous synthesis of the entire process, which can be extremely effective, as all elements of the system can be determined with regards to the entire process. However, the validity of the solution is significantly dependent upon the detail of the model formulated to simulate the superstructure. The geometrical approach is founded upon the attainable region (AR) theory, which was developed to

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http://dx.doi.org/10.1016/J.ENG.2017.02.008
2095-8099/

take into account the effect of having multiple interacting reactors and external heat exchangers [3]. The combined-targeting approach employs elements from both of the aforementioned techniques, as it stems from both the superstructure approach and the AR theory. Both the geometrical and the combined-targeting approaches incorporate the AR theory, limiting their utility. This is due to the fact that the AR theory integrates technical criteria, such as conversion and selectivity, as opposed to financial criteria; as a result, the solution may not be optimal from an economic standpoint. Bedenik et al. [2] have developed a novel technique to solve reactor network problems; this technique uses the superstructure approach and reformulates it to focus on the financial criteria of the model, including the impact of economic uncertainty over time, an aspect that will be discussed further in this report. Their technique is therefore more likely to be able to successfully find the optimal configuration, although it requires a thoroughly detailed mathematical model.

The vast majority of problems related to the field of process systems engineering involve continuous as well as discrete decisions. Typically, discrete decisions account for the underlying logic of the process, such as selection of a reaction pathway or expansion of capacity for planning problems, while continuous decisions account for product flow rates, amount of sales, and so forth. In order to mathematically model these kinds of decisions, continuous as well as 0–1 integer variables are employed, thus resulting in mixed-integer programming (MIP) problems. For a case in which the governing laws are expressed through nonlinear relations, the resulting problem is a mixed-integer nonlinear programming (MINLP) problem, which can generally be formulated as follows [1]:

$$
\begin{aligned}
& z^* = \min_{x,y} f(\boldsymbol{x}, \boldsymbol{y}) \\
\text{s.t.} \quad & \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{y}) \le 0 \\
& \boldsymbol{x} \in X \subseteq \mathbb{R}^{n_x},\ \boldsymbol{y} \in Y = \{0,\ 1\}^{n_y}
\end{aligned} \tag{1}
$$

where f is a scalar function; $\boldsymbol{x}$ is the n_x-dimensional vector of continuous variables that belongs to the bounded set X; $\boldsymbol{y}$ is the n_y-dimensional vector of binary variables that belongs to the discrete set Y; $\boldsymbol{g}$ is the vector of constraints that accounts for quality bounds, demand satisfaction, and so forth; and z^* refers to the optimal solution of the optimization problem.

Because of their generic mathematical nature, MINLP problems have found application in a wide scope of problems such as process synthesis of reactor networks [4], HENs [5], process planning, and enterprise-wide optimization of manufacturing processes [6], to name just a few. Process synthesis forms a fundamental class of MINLP problems in the area of engineering, in which simultaneous decisions on the selection of processing units, interconnections, and design/operating variables need to be made [7]. Despite MINLPs' ability to mimic the system under study more accurately than their linear counterparts (mixed-integer linear programming, MILP), these problems are difficult to solve because of the possible non-convexities that arise [8]. A number of numerical techniques have been proposed in the open literature to solve certain classes of MINLPs, such as the generalized Benders decomposition (GBD) [9], the outer approximation (OA) algorithm [10], and extended cutting plane (ECP) methods [11]. The aforementioned algorithms can be used in a rigorous manner under specific assumptions about the convexity of the objective function and the form of nonlinearities involved, while an iterative procedure is generally followed to typically converge to a (locally) optimal solution. Another class of MINLP solution algorithms falls under the scope of global optimization [12,13], in which specialized numerical techniques and convex approximations are employed so as to solve the corresponding problem within a tolerance of ε-optimality.

In principle, the solution of MINLPs can be computationally demanding, even for a case in which no uncertainty is considered. However, mathematical models are susceptible to a number of uncertainties that can be broadly categorized as endogenous and exogenous [14]. Endogenous uncertainty is mostly encountered on the left-hand side of the constraints, such as reaction yields and stoichiometric coefficients, while exogenous uncertainty is usually located on the right-hand side (RHS) of the constraints and in the objective function coefficients (OFCs). In order to handle uncertainty within optimization problems, a number of solution techniques have been proposed in the literature; the main techniques are stochastic programming, robust optimization, and (multi-)parametric programming (mp-P) [15]. While the first two techniques require the availability of some form of data that can be used to characterize the uncertainty, such as probability distributions or type of uncertainty set, mp-P makes direct use of the mathematical model and, with optimization-based methodologies, aims to explicitly characterize the effect of the uncertainty on the optimal solution. Through the solution of an mp-P problem, one generally aims to compute the optimization variables as explicit functions of the uncertain parameters, along with the corresponding regions—that is, critical regions (CRs)—of the parametric space where each function remains optimal. Fig. 1 provides a conceptual graph of such a problem.

Having been studied for over 30 years [15,16], mp-P stands on solid theoretical foundations, with algorithms for every class of optimization problem. However, despite the constant developments in the field of mp-P, the class of (multi-)parametric (mp)-MINLPs remains among the least studied, even for a case in which only RHS uncertainty is considered. The reason for this lack of research is the non-convexity that is involved in the solution of the underlying parametric optimization problems. Early works focused on the approximate solution of single parametric MINLPs (p-MINLPs) [17–21], while Dua and Pistikopoulos [22] studied the mp-MINLP case with convex objective functions and proposed a decomposition approach in which successive iteration occurred between primal and master problems for the generation of valid upper and lower bounds, respectively. In their approach, the primal problem is an mp-nonlinear programming (mp-NLP) problem derived by fixing the related integer variables, while the master sub-problems aim to provide improved integer solutions. Dua et al. [23] studied the global optimization of mp-MINLPs. Polynomial parametric optimization techniques using algebraic geometry techniques were presented in Ref. [24], in which cylindrical algebraic decomposition and Gröbner

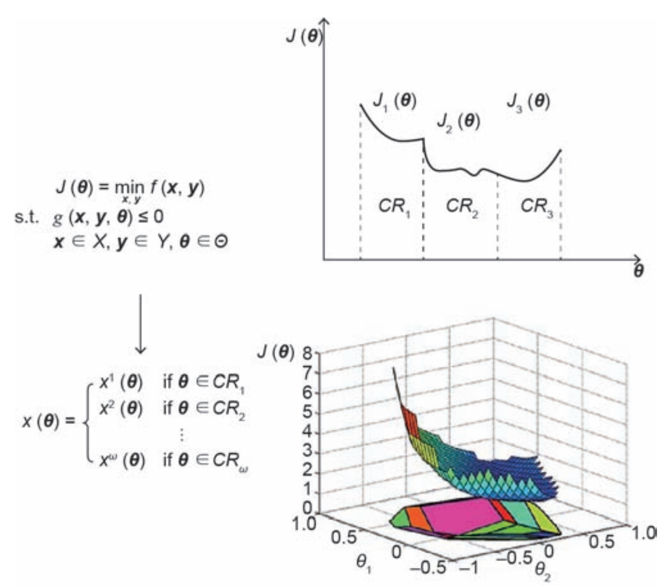

Fig. 1. Conceptual graph of the mp-P scope.