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A Methodology for the Approximate Stochastic Synthesis of Flexible Chemical Processes

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Abstract

This work presents a two-level methodology for the optimal design and MINLP synthesis of flexible chemical processes with known probability distributions of uncertain parameters. This methodology comprises synthesis at 1) nominal level and 2) approximate stochastic level. Both levels rely on considerable reduction of discrete points. The first level provides good starting and flexible structure for the second level, therefore, the computational effort is reduced and larger problems with many uncertain parameters, e.g. 10 to 100, can be solved. The use of this methodology is illustrated by the synthesis of a flexible heat-integrated methanol process flow sheet.

Keywords: process design, synthesis, flexible, stochastic, uncertain, MINLP

1. Introduction

The design and, in particular, the synthesis of large flexible process flow sheets with a significant number of uncertain parameters is still a challenging problem. The main reason is that such problems are usually solved by the discretization of an infinite uncertain space, which may cause an enormous increase in a problem's size. Several authors have proposed various approaches for facilitating the process synthesis under uncertainty [1-3]. However, a step forward should be taken in order to relate flexible synthesis to real-size applications. The main purpose of this contribution is to develop a robust and reliable strategy for the MINLP synthesis of flexible process flow sheets, which can solve those larger synthesis problems having a considerable number of uncertain parameters. This approach can also be applied to NLP design when process flowsheets are considered at fixed topology.

2. Methodology description

The main idea is to perform the synthesis through several levels, from a less accurate simple level to more accurate, approximative stochastic level, which is computationally more demanding. As the first level generates a good initial structure for the second level, the latter needs less iterations and the computational effort can be significantly reduced.

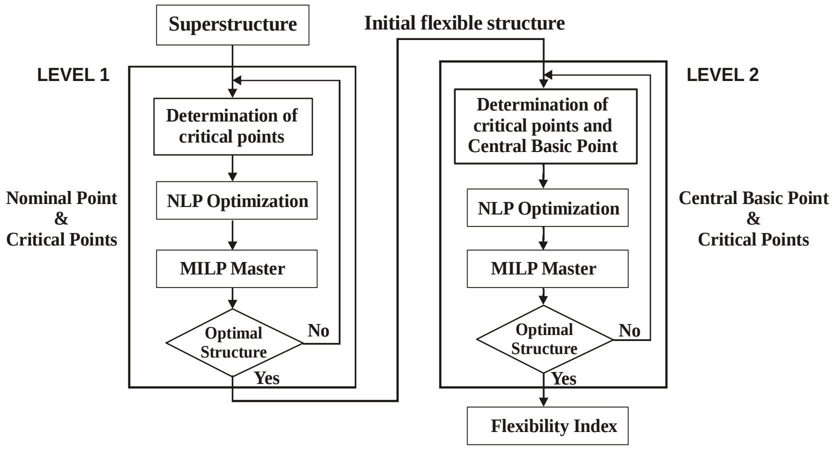
2.1. Two-level MINLP synthesis for flexible flow sheets

The flexible synthesis is performed at both levels simultaneously at several critical points, θ_c, $c \in CP$, and at one point, θ_{ap}, which is used for approximating the objective function's expected value. The latter is usually rather close to the objective value obtained at the nominal point. Therefore, the objective function at the first level is evaluated simply at the nominal values of uncertain parameters, $\theta_{\mathrm{ap}}=\theta^{\mathrm{N}}$. At the second level, the central basic point [4] takes this role in order to account for possible deviations in the expected value from the nominal point, $\theta_{\mathrm{ap}}=\theta^{\mathrm{CBP}}$. The central basic point is determined through one-dimensional Gaussian integration, which will be described in Section 2.3.
The mathematical problem for flexible MINLP synthesis either at the first or at the second level has the following form:

$$
\begin{aligned}
&\min_{y,x_{\mathrm{ap}},z_{\mathrm{ap}},d} C(y,x_{\mathrm{ap}},z_{\mathrm{ap}},d,\theta_{\mathrm{ap}}) \\
&\text{s.t.} \\
&h(y,x_{\mathrm{ap}},z_{\mathrm{ap}},d,\theta_{\mathrm{ap}})=0 \qquad h(y,x_c,z_c,d,\theta_c)=0 \\
&g(y,x_{\mathrm{ap}},z_{\mathrm{ap}},d,\theta_{\mathrm{ap}})\le 0 \qquad g(y,x_c,z_c,d,\theta_c)\le 0 \qquad c\in CP \qquad \text{(P1)} \\
&d \ge g_d(x^{\mathrm{ap}},z^{\mathrm{ap}},\theta^{\mathrm{ap}}) \qquad d\ge g_d(x_c,z_c,\theta_c) \\
&x_{\mathrm{ap}},z_{\mathrm{ap}},x_c,z_c,d\in R,\ y\in\{0,1\}^{\boldsymbol{m}},\ \theta^{\mathrm{LO}}\le\theta_c\le\theta^{\mathrm{UP}},\ \ \theta_{\mathrm{ap}}=\theta^{\mathrm{N}} \text{ or } \theta^{\mathrm{CBP}}
\end{aligned}
$$

In the model (P1), $\boldsymbol{y}$ represents vector of binary variables for the selection of process topology. $\boldsymbol{x}$, $\boldsymbol{z}$ and $\boldsymbol{d}$ are the vectors of the state, control and design variables (sizes of process units), respectively. C is the economic objective function, $\boldsymbol{g}$ and $\boldsymbol{h}$ are the vectors of (in)equality constraints and $\boldsymbol{g}_{\mathrm{d}}$ represents the design specifications. The left group of constraints represents the optimization at the single point, θ_{ap}, which approximates the expected objective function. The right group of constraints refer to the critical points, θ^{c}, from the set, *CP*. These points are always presented in synthesis models, as they assure sufficient sizes of process equipment for feasible operation. They have to be determined in advance for each flow sheet selected by the optimization algorithm, as will be described in the next subsection. Flexible synthesis is then performed by means of an MINLP algorithm, e.g. Outer Approximation/Equality Relaxation algorithm (Fig. 1).

Fig. 1. Two-level strategy for flexible MINLP synthesis



2.2. Determination of critical points

Critical points in this work are defined as those combinations of uncertain parameters that require the largest overdesign of process units for given deviations of uncertain parameters. Equipment dimensions have to suit all predefined deviations at minimum cost. This means, that the flexibility index of the optimal flexible solution, as defined in the literature [5], has to be equal or very close to 1. In our recent work [6,7], we proposed various schemes for identification of critical points, however, it has emerged during this work that simplified noniterative formulation is, for now, the most appropriate for large process flow sheets.

This formulation is mathematically described by a non-linear model (P2) where the binary variables are fixed, y^{fx}, according to the temporarily selected flow sheet structure. Uncertain parameters are transformed into variables that can vary between the selected lower and upper bounds, θ^{LO} and θ^{UP}.

Assume that the number of design variables in particular structure is n_d. Then, NLP problem (P2) is solved for n_d-times by searching for the maximum value of each design variable d_i, at minimum cost. This is achieved by subtracting the design variable multiplied by a large scalar M, from the cost function C. The result of n_d subproblems are the critical values of uncertain parameters which are then merged into the smallest set of critical points.

$$
\begin{aligned}
&\min_{x,z,d,\theta} C(y^{fx}, x, z, d, \theta) - M \cdot d_i \\
&\text{s.t.} \quad h(y^{fx}, x, z, d, \theta) = 0 \\
&\qquad g(y^{fx}, x, z, d, \theta) \le 0 \\
&\qquad d = g_d(x, z, \theta) \\
&\qquad \theta^{LO} \le \theta \le \theta^{UP} \\
&\quad x, z, d, \theta \in R,\ y^{fx} \in \{0,1\}^m
\end{aligned}
\qquad \begin{matrix} (P2)_i \\ i=1,2,\ldots,n_d \end{matrix}
$$

2.3. Determination of central basic point

The determination of the central basic point was extensively described in our previous work [4]. In order to summarize the procedure briefly, it should be emphasized that coordinates of this point are determined by one-dimensional stochastic integration of each uncertain parameter over its Gaussian quadrature points. In this integration the remaining uncertain parameters are held at their nominal values while the critical points are included to assure flexibility. Objective values obtained at five Gaussian points are fitted into the curve which correlates values of particular uncertain parameter with the objective function values. The basic coordinate is then determined from this curve as the value of uncertain parameter at which the optimal objective function is equal to the expected objective function determined during one-dimensional integration. The basic coordinates of all uncertain parameters constitute a vector of central basic point which is used for the approximation of the expected objective function.

3. Synthesis of flexible heat-integrated methanol process

This methodology was applied for the synthesis of a flexible heat-integrated methanol process (Fig. 2) where methanol is produced from hydrogen and carbon oxide. This example was taken from the literature [8] and the prices were updated. This flow sheet is medium-sized with 32 streams, 4 hot and 2 cold process streams. Eight binary variables were used for selection between two feed streams, between one- or two-stage compression of the feed stream, two reactors, and one- or two-stage compression of the recycle stream. Additional 38 binary variables were assigned for the selection of heat matches between process streams, as well as between process streams and utilities in the four-stage MINLP heat-integration superstructure [9].

24 uncertain parameters were defined with nominal values and deviations: annual production, temperatures, pressures, compositions and the prices of the feed streams, product, electricity, steam and cooling water, heat transfer

coefficients, conversion parameters in the reactors and efficiencies of the compressors.

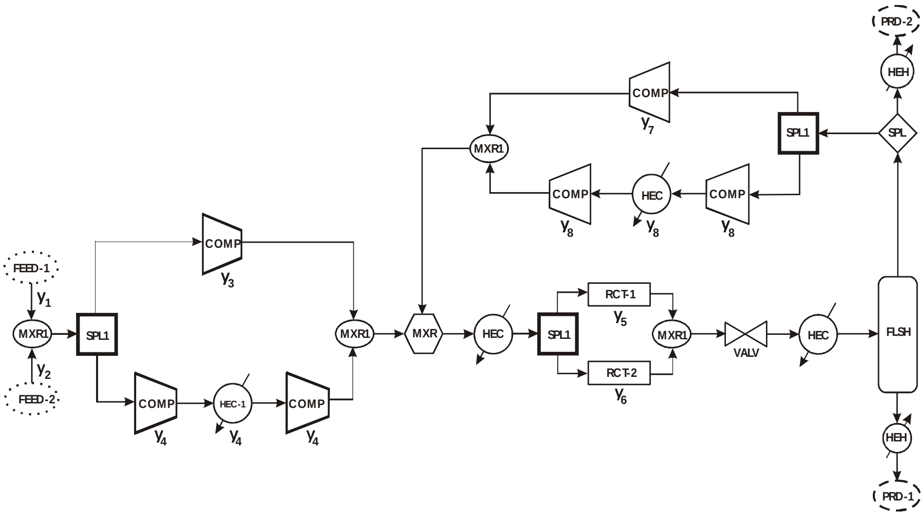


Fig. 2. Methanol process superstructure

3.1. Deterministic non-flexible synthesis

Deterministic synthesis at the nominal values of uncertain parameters with no flexibility consideration yielded a solution with a profit of 37.37 MUSD/yr. The optimal structure was comprised of more expensive feed stream (FEED-2), double-stage feed compression, cheaper reactor with lower conversion (RCT-1), and one-stage recycle compression. This structure is a threshold problem with two process heat exchangers, two coolers, and no heaters. It was determined that even small deviations in the uncertain parameters from the nominal values result in infeasible solutions.

3.2. Nominal flexible synthesis

Flexible synthesis was performed at the nominal point and at the critical points. MIPSYN, an MINLP process synthesizer with a modified OA/ER algorithm [10] was used to perform five MINLP iterations yielding the same optimal topology than deterministic synthesis. The profit was significantly reduced to 33.04 MUSD/yr, mostly because of larger compressors on the feed stream, a larger reactor, and some exchangers. However, flexibility index of this solution was determined for deviations of influencing uncertain parameters yielding a value of 1.004, which indicates a flexible solution. Optimal design was tested by applying Monte Carlo simulation over 4000 randomly selected points that assure the mean value within an error of ±0.23 MUSD/yr at 95 % confidence limit. The expected value obtained with Monte Carlo was 32.82 M$/yr which indicates that the nominal result (33.04) is within required confidence interval.

3.3. Approximate stochastic flexible synthesis

In this MINLP step, the normal distributions of uncertain parameters were defined with mean values equal to the nominal values and total deviation intervals equal to six-times standard deviations (6σ). The central basic point was determined for the optimal structure obtained at the previous level and the synthesis started at this point, and at the critical points. The approximated expected profit of the optimal structure is 32.72 MUSD/yr. The values of the design variables were close to those obtained using the nominal approach. Monte Carlo simulation yielded the expected profit of 32.81 MUSD/yr. This may indicate that, in the case of normal distributions of uncertain parameters, nominal point could give sufficiently accurate approximation of the expected value and exhaustive stochastic optimizations can thus be avoided.

4. Conclusions

A strategy is presented for the MINLP synthesis of flexible process flow sheets with many uncertain parameters. The procedure is evolutive and progresses from simple, less accurate steps to more demanding, but more accurate steps. The lower levels assure good initial flexible structures for higher levels which then converge faster. Moreover, it is expected that in many cases optimal topology could be found at the lower level, while at the upper level only fine adjustments of the design variables and the expected objective value are performed. A further motivation is thus to improve methodology in order to obtain flexible process flow sheets in just a few iterations.

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