# A STRATEGY FOR MINLP SYNTHESIS OF FLEXIBLE AND OPERABLE PROCESSES

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*Abstract*

This paper presents a sequential two-stage strategy for the stochastic synthesis of chemical processes in which flexibility and ability to adjust manipulated variables are taken into account. In the first stage, the optimal flexible structure and optimal oversizing of the process units are determined in order to assure feasibility of design for a fixed degree of flexibility. The feasibility is assured by simultaneous consideration of critical vertices while the expected value of the objective function is approximated by the optimization at the base point. The latter is determined by a simple set-up procedure based on the calculations of the objective function's conditional expectations for uncertain parameters. In the second stage, the structural alternatives are included in the mathematical model in order to introduce additional degrees of freedom for efficient control. This strategy is illustrated by two examples for heat exchanger network synthesis and can also be applied to other process subsystems.

*Keywords*

Synthesis, MINLP, Operability, Flexibility, Controllability, Steady State Model

## Introduction

During the last few decades, mathematical programming has proved to be excellent tool for design, synthesis and retrofit of chemical processes and numerous methods have been successfully implemented into the existing CAPE (Computer Aided Process Engineering) tools. In order to approach the solutions obtained by means of these methods to the plants that are actually implemented in practice, operability issues (like flexibility, controllability, reliability, safety) should be considered during the design, synthesis and retrofit of chemical processes. Recently, there have been many attempts to introduce operability aspects into those systematic methods from which flexibility has been most widely addressed (see e.g. Acevedo and Pistikopoulos, 1998).

Interactions between process design and process control have been shown to have a great impact on the economic optimality of a process design. Kotjabasakis and Linnhoff (1986) introduced sensitivity tables for the design of flexible processes. Mathisen (1994) investigated design and control of heat exchanger networks. Several authors have developed systematic methods for the synthesis of process schemes, which are flexible to operate under uncertain conditions and operable for a disturbances (Papalexandri and Pistikopoulos, 1994; Glemmestad et al., 1997; Mizsey et al., 1998; Tantimuratha et al., 2001).

In this paper, a sequential two-stage approach is presented for the synthesis of flexible and operable processes by means of mixed-integer nonlinear programming (MINLP). In the first stage the selection of optimal process topology is performed together with determining the optimal oversizing of process units to assure the desired flexibility. In the second stage the optimal selection of additional structural alternatives and manipulated variables is performed in order to assure efficient control. This paper is organized as follows: firstly, a simplified set-up procedure for the selection of a basic point is proposed, and secondly, a two-stage strategy is described by which a steady-state mathematical model is developed for process control. Two examples are presented to illustrate this two-stage synthesis. It is assumed in this paper that the maximum variations and distribution functions of the uncertain parameters are known and that a feasible solution can be obtained for every realization of uncertain parameters.

**Set-up Procedure for Basic Point**

Uncertainties are often described by means of normal and uniform distributions, which are both symmetrical. However, from the practical point of view, skewed distributions are more realistic. Beta distribution is a type of probability distribution defined on a finite interval which may have its modal value anywhere in the interval. The approximate density function can be obtained by estimation of only three values: lower bound, $a$, upper bound, $b$ and mode, $m$ – the most probable value. For that reason, the uncertain parameters in this work are described by beta density functions.

The main problem of stochastic optimization is accurate estimation of the expected objective function that requires discretization and exhaustive computations at numerous quadrature points. The RDS method (Novak and Kravanja, 1999) approximates the expectation by a linear combination of objective values in a reduced set of extreme points (basic vertices) determined in the preceding set-up procedure. The drawback of this method is that the selection of basic vertices in the set-up procedure is not unique and many suboptimal solutions can be generated. The aim of this work is to simplify and to modify the set-up procedure so that more accurate approximation of the expected value can be obtained.

The main idea of the proposed procedure is to determine just one central basic point in which the value of the objective function would be close to the expected value of the objective function. The central basic point is determined in the following way. First, conditional expectations of the objective function for each uncertain parameter, $\theta_i$, have to be obtained. They are estimated over a significantly reduced region by Eq. 1, which requires optimization of the problem simultaneously in $n$ quadrature points for a given uncertain parameter, while other uncertain parameters are held at the modal values ($\theta_j^m$).

$$EC(\theta_i) = E\left[C(\theta_i)\middle|\theta_j = \theta_j^{\mathrm{m}}, j = 1,2,\ldots,N \wedge i \neq j\right] = \sum_{k=1}^{n} C(\theta_{i,k}) \cdot v_{i,k} \qquad i = 1,2,\ldots,N \tag{1}$$

where $v$ represents coefficients obtained from the density function and points $\theta_{i,k}$ correspond to $n$ quadrature points determined as zeros of the Legendre polynomial. When calculating the conditional expectations, the feasibility constraints should be considered simultaneously in vertices that require the largest overdesign of process units (critical vertices – $CV$). Critical vertices are determined by the preceding scaning of extreme points.

Based on the realizations of the objective function $C_k$ at the $n$ points the approximate functions $C(\theta_i)$ are developed for each uncertain parameter $\theta_i$ by a simple curve fitting. From these functions it is then possible using a simple back calculation to predict the values of uncertain parameters ($\theta_i^{\mathrm{E}}$) which would produce values of the objective function equal to the values of the corresponding conditional expectations:

$$C(\theta_i^{\mathrm{E}}) = EC(\theta_i) \qquad i = 1, 2,\ldots,N \tag{2}$$

A vector $\theta^{\mathrm{E}}$ is determined by applying Eq. (2) for all uncertain parameters and serves as a basic point ($BP$) at which the expected value over the whole region of uncertain parameters can finally be approximated as $EC(\theta^{\mathrm{E}})$. In this way the expected value is determined at one basic point rather than at many as in the RDS method, and even approximates expected value more accurately.

**Two-stage Strategy for Flexibility and Operability**

Two important facts should be considered when performing synthesis of flexible and controllable process schemes: first, the process units should be properly oversized to assure the desired flexibility and second, the process structure should have sufficient degrees of freedom for efficient control.

*First Stage – Flexibility*

In the first stage the MINLP model (P1) is solved simultaneously in the union of critical vertices and basic point:

$$\begin{aligned}
&\min_{y_{\mathrm{t}},x,z,d} \; c_{\mathrm{t}}^{\mathrm{T}} y_{\mathrm{t}} + f(y_{\mathrm{t}}, x_i, z_i, d, \theta_i)_{i\in BP} \\
&\text{s.t.} \quad \left.\begin{aligned} & h_i(y_{\mathrm{t}}, x_i, z_i, d, \theta_i) = 0 \\ & g_i(y_{\mathrm{t}}, x_i, z_i, d, \theta_i) \le 0 \\ & d \ge g_{\mathrm{d}}(x_i, z_i, \theta_i) \end{aligned}\right\} i \in CV \cup BP \\
&\qquad\quad d \ge d^{\mathrm{LO}} \\
&x \in X,\ z \in Z,\ d \in D,\ y_{\mathrm{t}} \in \{0,1\}^{m_{\mathrm{t}}} \\
&\qquad \theta \in TH,\ BP = \left\{\theta^{\mathrm{E}}\right\}
\end{aligned} \tag{P1}$$

$x$, $z$, $d$ and $y_{\mathrm{t}}$ are the vectors of process, control, design and topology binary variables, respectively, and $\theta$ is the vector of uncertain parameters. $h$ and $g$ are vectors of equality and inequality constraints, while $g_{\mathrm{d}}$ represents the terms by which design variables are defined. The objective function $f$ represents the approximation of the expected economic criteria calculated at $\theta^{\mathrm{E}}$. Fixed costs associated with process topology, $c_{\mathrm{t}}$, can also be included.

Since in this work we deal with one single basic point instead of many quadrature points the economic trade-off over the entire uncertain space is not considered and P1 would produce optimistic results. Therefore, the approximate trade-off is introduced in problem P1 by setting lower bounds on design variables ($d^{\mathrm{LO}}$). The bounds are obtained through calculations of the conditional expected values for each uncertain parameter over one-dimensional space by Eq. 1. Maximal values of design variables obtained in this way are stated as lower bounds in MINLP optimization for the determination of optimal flexible structure. It is assumed that 'conditional overdesign' obtained in this way is the approximation of overdesign that would be obtained by simultaneous optimization at quadrature points.

Optimization of problem (P1) yields solutions with optimal process structure and optimally oversized design variables which enables the desired flexibility of process schemes.

*Second Stage – Operability*

The structures obtained by solving problem (P1) may, in general, possess an insufficient degree of freedom to assure effective process control. In order to add missing degrees of freedom, additional structural alternatives should be introduced into the process scheme together with additional manipulated variables (e.g. bypasses in heat exchangers). In the same way the model (P1) is reformulated. This can be achieved by assigning one or more additional manipulated variables ($z^a$) to each design variable. Oversizing of design variables is sufficient for some realizations of uncertain parameters and an additional manipulated variable is not needed ($z^a$=0). For other realizations the oversizing could be excessive ($z^a$>0). Manipulated variables are included to compensate for the difference between the oversized and actually required values of the design variables at a particular point which represents the additional degrees of freedom.

In the reformulated model (P2), the design terms are written as equalities, and binary variables are introduced for the selection of additional manipulated variables, $y_z$. The optimal selection of additional structural alternatives and manipulated variables is determined for optimal flexible topology ($y_t$*) from the first stage:

$$\min_{y_z, x, z, z^a, d} c_t^T y_t^* + f(y_t^*, x_i, z_i, z_i^a, d, \theta_i)_{i \in BP} + c_z^T y_z$$

$$\text{s.t.} \left. \begin{aligned} & h_i(y_t^*, x_i, z_i, d, \theta_i) = 0 \\ & g_i(y_t^*, x_i, z_i, d, \theta_i) \le 0 \\ & d = g_d(x_i, z_i, \theta_i) + \Delta g_d(x_i, z_i^a, \theta_i) \end{aligned} \right\} i \in CV \cup BP$$

$$z_i^a \le U y_z \qquad \text{(P2)}$$

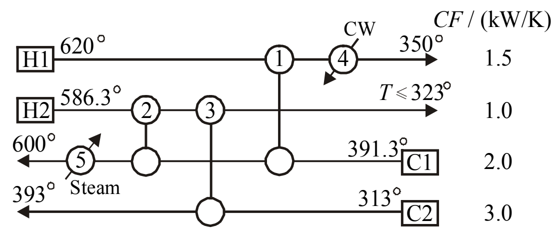
$$x \in X,\ z \in Z,\ d \in D,\ y_z \in \{0,1\}^{m_z}$$

$$\theta \in TH, BP = \{\theta^E\}$$

If the introduction of additional manipulated variable requires an additional structural alternative, fixed costs $c_z$, are included in the objective function. $U$ is a large positive constant in a logic relationship for potential (non)existence of an additional manipulated variable. If an alternative is required at the particular point, its binary variable ($y_z$) is set to 1 and the logic relationship allows a nonzero value for the manipulated variable.

**Illustrating Example**

The methodology is outlined on the small HEN example. The uncertain parameters are the inlet temperatures of cold stream C1 and hot stream H2 and the heat capacity flow rate of cold stream C2. The lower, modal and upper values [$a$, $m$, $b$] are given as follows: $T_{IN,C1}$ [378, 391.3, 398], $T_{IN,H2}$ [573, 586.3, 593], $CF_{C2}$ [2.9, 3.03, 3.1]. The mathematical model comprises heat balances, the restrictions on temperatures and the expressions for heat transfer area. The objective is to minimize the sum of annual investment and operating cost. A fixed structure as shown in Figure 1, was used for this example to shorten the first synthesis step.




Cost of exchangers and coolers ($/yr): 1846 $A^{0.65}$
Cost of heaters ($/yr): 2350 $A^{0.65}$ ($A$ in $m^2$)
Cost of CW: 20 $/(kW yr)
Cost of Steam: 80 $/(kW yr)

*Figure 1. Heat exchanger network of illustrating example*

*Set-up procedure and stochastic optimization (P1)*

The example is used to illustrate the proposed set-up procedure to evaluate the basic point at which model (P1) is solved to approximate the expected value of the objective function. First, conditional expected values and functions $C(\theta_i)$ are determined for each uncertain parameter from which a basic point $\theta_i^E$ is determined ($T_{IN,C1}$=388.87 K, $T_{IN,H2}$=584.63 K, $CF_{C2}$=3.045 kW/K). The problem (P1) is then solved at this basic point subject to the flexibility constraints defined at the two critical vertices. Minimal cost obtained (45825 $/yr) is similar to the one for the stochastic solution obtained simultaneously at 125 quadrature points (45700 $/yr).

*Second stage (P2)*

In the second stage, the HEN structure is extended by new structural elements from which manipulated variables are introduced to the problem. In this case three bypasses are added on the cold streams of process exchangers (1, 2 and 3) as structural alternatives while the fractions of bypassed streams are corresponding manipulated variables. The choice of bypass placement is arbitrary because a steady state model is applied. Three binary variables are introduced for bypasses and charged by fixed cost (1300 $/yr) in the objective function. The structure was tested over the region of possible deviations. Controllability was proven only when there was no restriction on the fractions of the bypassed streams.

However, in practice the bypasses are limited by some upper bounds, which reduces operability. Hence, additional degrees of freedom have to be introduced in the structure: an additional cooler is placed on the hot stream H2 and an additional heater on the cold stream C2 and charged properly in the objective function. In this way a trade-off between bypass placement and utilities consumption is introduced into the optimization and a new superstructure of problem P2 is thus generated. The mathematical model of this superstructure comprises 5 binary variables ($y_z$ in P2): three for bypasses and two for additional heater and cooler.

The upper limit of the bypassed streams is fixed to 30 % of the total heat flow rate. The conditional expectations are calculated for three uncertain parameters (47804, 48008, 48019) $/yr and the basic point is determined to be (389.85 K, 584.79 K, 3.046 kW/K). MINLP optimization of the extended superstructure at the basic point with flexibility constraints in two critical vertices yields the structure shown in Fig. 2 and the expected cost of 48402 $/yr. The expected cost is higher than the one of the first stage (45825 $/yr) because the optimal solution (Fig. 2) additionally comprises two bypasses and one heater on cold stream C2 and some additional heating utility.

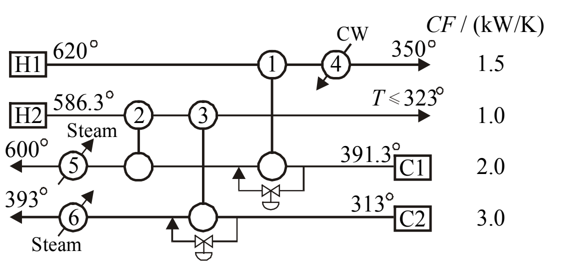



*Figure 2. Optimal flexible and operable heat exchanger network of the illustrated example*

This problem is also solved simultaneously at 125 Gaussian quadrature points yielding the solution 48430 $/yr which indicates that good approximation of the expected value was obtained by the proposed procedure.

## Example of HEN Synthesis

The example of HEN synthesis with three hot and four cold streams was considered in this section (Yee and Grossmann, 1990). An optimal nonflexible structure comprises 5 exchanger units, one cooler and one heater. Its cost amounts to 158 k$/yr. 6 uncertain parameters were defined: inlet temperatures of two streams, heat capacity flow rate of one stream, prices of cooling water and steam and heat transfer coefficients. It should be noted that economical uncertain parameters (prices) have an influence on the synthesis of optimal structure and determination of optimal oversizing, while uncertain process parameters are important for the control.

In the first stage, optimal topology was determined comprising 6 exchanger units, one cooler and one heater. Total expected cost of the flexible structure is 176 k$/yr. In the second stage, bypasses are added to the exchangers and additional heaters and coolers on the streams in order to obtain sufficient degrees of freedom for control. The upper limit of fractions of bypassed streams was fixed to 22 %. The final structure obtained comprises 6 exchanger units from which 4 have bypasses. Heaters are placed on all cold streams and coolers on all hot streams. Annual cost of flexible and operable structure amounts to 229 k$/yr.

## Conclusions

The proposed strategy enables the synthesis of optimal process structures which are flexible for a given range of uncertainty, and operable for disturbances. The aim is to bridge the gap between the synthesis and the final operation of flexible and on-line optimized processes.

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