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Stochastic and hybrid approaches to solve integrated synthesis and operation of batch processes

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Abstract

This work aims at exploring two solution strategies to tackle the problem of simultaneous batch process synthesis and operational design, represented as a mixed-integer dynamic optimization (MIDO). A stochastic and a hybrid approach are presented, which are meant to keep the optimum solution performance while seeking for faster solutions and the capability of solving industrial sized problems. Specifically, a genetic algorithm (GA) and its combination with deterministic NLP solvers (GA-NLP) are developed and tested. The core idea in both alternatives is to combine in the GA chromosome a myriad of variables corresponding to the different kinds of decisions characterizing the problem solution, in order to reduce the combinatorial explosion to be managed by the standard NLP/MINLP solver. The decisions included are dynamic control profiles, time-invariant controls, and integers. Comparative results of the two strategies with respect to the purely deterministic solution are presented.

Keywords: batch process synthesis, operational design, differential GA, hybrid method.

1. Introduction

Nowadays, chemical industry faces tight and changing production frameworks, which usually require the introduction of new or modified products into existing manufacturing facilities. In this context, batch processes are very suitable due to their inherent flexibility and adaptability, and batch process synthesis is a key problem to develop effective and efficient processes (Rippin, 1993). However, fixed processing recipes, which are based on nominal conditions and tests in the laboratory or pilot plant, are usually employed. Additionally, further integration of operational decisions has been scarcely addressed, even though it could guarantee fully functional and optimally operated process plants in both nominal regimes and changing scenarios.

The problem of simultaneous batch process synthesis and operational design in existing plants is posed as a key problem for plant and process redesign and modernization. This problem may be challengingly represented as mixed-integer dynamic optimization (MIDO) models, which allow to combine integer variables representing the qualitative information related to the synthesis problem, as well as differential-algebraic equations explaining the dynamic behavior of the batch process itself. However, the mathematical complexity and the size of the resulting models require the use of advanced computational tools to solve them. Specifically, the use of deterministic approaches is not a trivial task due to the highly non-linear, discrete, and highly combinatorial nature of the problem, even for reduced sized problems.

This work aims at exploring two solution strategies, which are an alternative to the deterministic approach, in order to tackle MIDO for integrated synthesis and operational design in given plants. This kind of alternative strategies has been already considered in other problems of process systems engineering area (Capón-García, 2011).

2. MIDO for batch process synthesis and operational design

Integrated batch process synthesis and operational design involves the selection of the required processing tasks and their sequencing to transform raw material into final products, together with the definition of dynamic control profiles, batch stages constituting each task, and their assignment to equipment units. Particularly, the synthesis decisions covered in this work are the equipment configuration (Y_{conf}), selected equipment pieces, task-equipment assignment and number of batches, all of them responding to a qualitative nature. Besides, the operational design, understood as the feed-forward control to define the batch process model, requires the use of dynamic decision profiles, such as input and output flow rates ($F_{j,in}$ and $F_{j,out}$) and temperature ($T_{j,ku}$) at each unit j and batch stage ku, as well as time-invariant decision variables, like processing times (t^f_k) at each batch stage k of the plant. All these decisions can be gracefully modeled combining the use of logics in general disjunctive modeling, and the representation of discrete events and differential equations in multistage models. The resulting MLDO may be afterwards relaxed into a MIDO.

3. Proposed solution strategies

A stochastic and a hybrid approach are proposed in this work, with the objective of keeping solution goodness while impelling faster resolutions and the possibility of solving larger dimension systems.

3.1. Stochastic method. Genetic algorithm (GA)

The stochastic method proposed is a differential genetic algorithm (GA) (Michalewicz, 1992) with both continuous and integer genes combined in the chromosome (Figure 1). In the first part of the chromosome (I), a gene is used to represent each dynamic control profile. For that, the infinite-dimensional control profiles are discretized. Their corresponding vector of approximations at finite temporal points $e \in \{1,\ldots N_e\}$ constitutes a gene of continuous values. The discretization is carried out in this work by orthogonal collocation on finite elements (Cuthrell and Biegler, 1989). The second part of the chromosome (II) contains the time-invariant control variables, which are also continuous variables. The last part of the chromosome (III) involves the integer decisions. In the retrofit process synthesis here addressed, with equipment structure selection, these integer can be reduced to plant configuration $Y_{conf} \in \{1,\ldots N_{conf}\}$. The remaining ones, such as selected processing units and unit-task assignments, may be derived from plant configuration by using algebraic equations; otherwise, they should be also included in the chromosome.

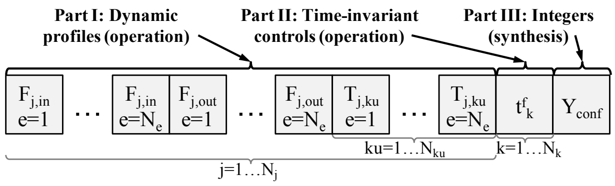

Figure 1: Representation of the chromosome for batch process synthesis and operational design.

The solution algorithm includes the following steps (Haupt and Haupt, 2004):

- **Initial population generation.** Random normalized values are assigned to each variable in the chromosome.

- **Fitness function evaluation and ranking selection.** After simulating the MIDO model for each chromosome and calculating the objective function, it is necessary to include some additional weights to penalize physical infeasibilities such as negative volumes or unaccomplished demand.
- **Replication of individuals by crossover and mutation operators.** Matchmaking is done using rank weighted random pairing. Besides, crossover is performed through cyclic chromosomes and an even number of crossover points. In continuous genes, the value at the two new offsprings is calculated from parents' genes by using heuristic crossover with a random repartition parameter. As for mutation, random normalized values are assigned, excepting input and output flow rates, with a random normally distributed mutation around the original value.
- **Termination.** The algorithm is stopped when no more improvement in evolution indicators, particularly in minimum and mean fitness function in two consecutive populations, together with achieving penalization of best individual under tolerance.

3.2. Hybrid method. Genetic algorithm and NLP combination (GA-NLP)

The hybrid approach is focused on exploiting the strengths of both stochastic GA and deterministic NLP solution tools. For that, as shown in Figure 2, an initial heuristic step is introduced to firstly fix integer decisions in the MIDO, and following solve a dynamic optimization (DO) with deterministic NLP solvers, and hence improving the performance over MINLP ones. In a first step (1), appropriate initial feasible solutions are obtained through a parallel GA with fixed configurations and constant control profiles in each batch stage instead of dynamic ones. These approximated solutions are included in a second GA (2), now incorporating dynamic profiles and free configuration. The obtained solution is improved in a final step (3) by using a NLP solver, fixing the integer part of the problem.

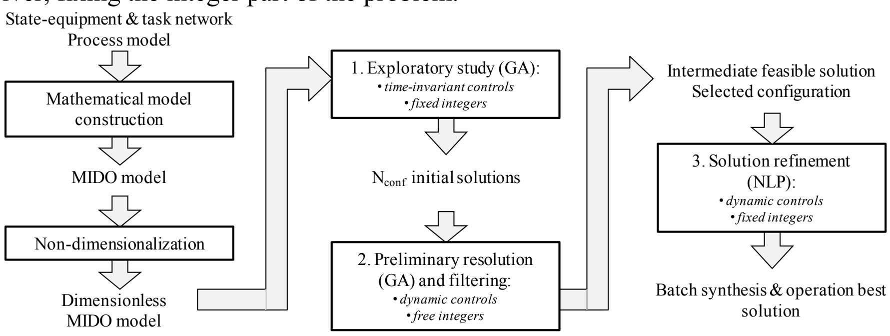

Figure 2: Proposed hybrid approach to solve batch process synthesis and operational design.

4. Example

The proposed strategies are applied to solve a batch retrofit synthesis and operational design problem in a single-product plant. The process consists of a network of two reactors where byproducts R, S, T and U may be obtained from raw material A through Denbigh reactions system. Further details may be found in Moreno-Benito and Espuña (2011). The objective is to produce 0.9 tons of S maximizing the profit (Eq. 1) with a product price of 6.15 €/kg S, raw material cost of 1.54 €/kg, fixed and variable processing costs of 99.98 €/h and 0.38 €/kg respectively in unit 1 and 199.96 €/h and 0.47 €/kg in unit 2.

$$Profit = Revenue_S - Cost_A - \sum_{j \in \{1,2\}} (Cost_{j,fixed} + Cost_{j,variable}) \quad (1)$$

4.1. Solution with genetic algorithm (GA)

In this example, a chromosome as the one presented in Figure 1 is employed, with N_j=2 units, N_{ku}=3 batch stages at each unit, N_e=4 finite elements for the discretization of batch profiles and using piecewise constant control profiles, and N_k=5 global batch stages. As a result, the chromosome length is 46, with 45 continuous and 1 discrete variables. An overview of GA features is shown in Table 1. To evaluate the goodness of each individual inside a population, the fitness function ($\Phi^{Fitness}$) is defined including the profit objective function ($\Phi^{Ojbective}$) and penalization of model unsupported restrictions (Eq. 2). In this example, penalizations P are committed to ensure: accomplished demand, minimum flow rates $F_{j,in}$ and $F_{j,out}$ in active units, zero volume in final time of each batch, lower and upper bound for stage times t^f_k and non-negative volumes in units and storage tanks. Penalization weights f_p should be sufficiently small to avoid converting any non-penalized (physically feasible) solution in a super-individual, but sufficiently large to avoid convergence towards penalized individuals with overrated profit.

$$\Phi^{Fitness} = \Phi^{Objective} + Penalizations = -Profit + f_p\ P \qquad (2)$$

Table 1: Genetic Algorithm parameters

Parameter		Parameter		Parameter		Parameters	
N. variables	46	Selection	50 %	N. crossover points	2	Mutation rate	5%
N. population	460	N. elite individuals	2	Penalization weight f_p	30	σ^2 in mutation ($F_{j,in}$ & $F_{j,out}$)	0.25

4.2. Solution with hybrid method (GA-NLP)

Steps 1 and 2 of the GA-NLP method (Figure 2) use the same GA features from Table 1. However, in the exploratory step there is one less variable Y_{conf}, which is fixed with four possible values: 1 and 2 for operation in one single reactor (unit 1 or unit 2 respectively), 3 for series, and 4 for parallel operation in both units. In step 3 (Figure 2), the NLP solver CONOPT is used.

4.3. Results

Evolution of fitness function obtained through the GA and hybrid GA-NLP strategies is shown in Figure 3, as well as the reference solution obtained with deterministic MINLP solver DICOPT, which uses outer approximation (OA) strategy.

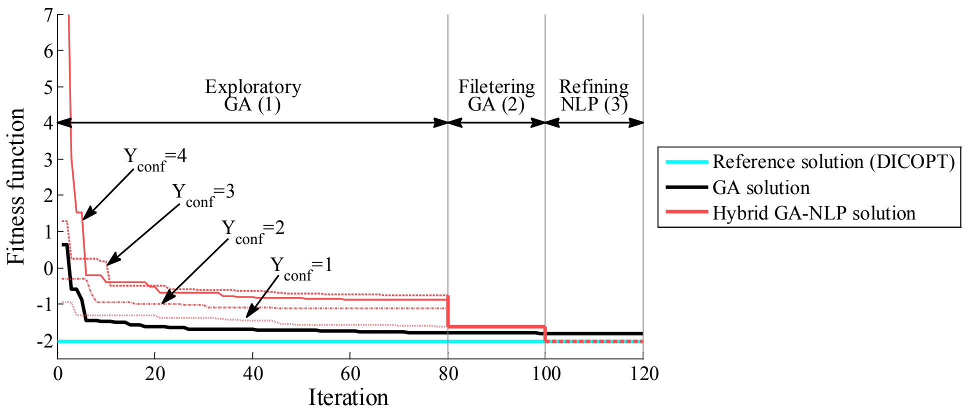

Figure 3: Evolution of the GA in the stochastic and the hybrid methods

The goodness of obtained solutions, which may vary in accordance to the GA tuning, is compared in Table 2 for the solution strategies proposed. It can be observed how the GA strategy provides a solution closer to the reference optimal one, in comparison to the hybrid strategy without refinement. Indeed, in the filtering GA (step 2) of the hybrid method, no improvement is obtained over the N_{conf} chromosomes provided from step 1, even though dynamic profiles are now allowed and provide a margin to solution improvement. A simple filter to automatically select the best out of the N_{conf} solutions available would be likewise appropriate. Besides, the almost negligible penalizations are common to all cases. Additionally, it is noteworthy how the GA strategy converges to a good solution as rapidly as exploratory GA in hybrid method (Figure 3); it should be equally efficient to solve a unique GA with free configuration and dynamic profiles, substituting steps 1 and 2, to afterwards refine the solution with a NLP solver in step 3.

Table 2: Comparison of solution goodness for the different strategies

Case	$\Phi^{Fitness}$	$\Phi^{Ojbective}$	$f_p\,P$	Error in $\Phi^{Fitness}$
OA reference	-2.0303	-2.0303	0	-
GA strategy	-1.8306	-1.9083	0.0777	0.1997
Hybrid: filtering GA	-1.6219	-1.6382	0.0164	0.4084
Hybrid: refining NLP	-2.0303	-2.0303	0	0

5. Conclusions

In this work, GA strategy and its combination with NLP is proved to be an alternative to deterministic MINLP solution in batch process synthesis and operational design. In the tested cases, physically feasible solutions are obtained without providing initial feasible solutions, which is a crucial advantage in front of deterministic methods. In the GA strategy, obtained solutions are close to the reference, and can be further improved up to the reference optimum by using NLP solvers with lower combinatorial complexity, as shown in the hybrid approach. These results are a promising first step to solve industrial size problems, currently limited by computational requirements of standard solvers.

Acknowledgements

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