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Optimization of a Large Scale Industrial Reactor Towards Tailor Made Polymers Using Genetic Algorithm

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Abstract: This paper presents a computational procedure for producing tailor made polymer resins, satisfying customers' needs while operating with maximum profit. The case study is an industrial large-scale polymerization reactor. The molecular properties considered are melt index (MI), which measures the molecular weight distribution, and stress exponent (SE), which is related to polydispersity. An economic objective function is associated to a deterministic mathematical model and the resulting optimization problem is solved by genetic algorithm (GA), a stochastic method. The GA parameters for both binary and real codifications are tuned by means of the design of experiments. Attempting to achieve the global optimum, a hybrid method, which introduces process knowledge into GA random initial population, is proposed. The binary codification performs better than the real GA, especially with hybridization. Results show that the GA can satisfactorily predict tailor made polymer resins with profits up to 25% higher than the industrial practice.

Keywords: polymerization, optimization, genetic algorithm, design of experiments, product design

1 Introduction

The thermal, mechanical, rheological and optical properties of a polymer are usually correlated with intrinsic properties such as average molecular weight, polydispersity and molecular weight distribution (MWD). Intrinsic properties, in their turn, depend heavily on reactor operating conditions. Reaction is therefore the key stage when designing polymer grades with controlled properties. Usually pilot plant or industrial scale experiments are carried out for this purpose. However, such practices are imprecise, time-delayed and lead to off-spec products and high costs. The development of computer-based tools has led to a reduction in this empiricism by means of simulation and optimization studies. Within this scope, the present study proposes an optimization problem for targeting polymer resins for an industrial scale process.

In the last years much attention has been given to the design of tailored polymer resins through optimization models. Most research focuses on batch polymerization and then minimizes the batch time while specifying the polymer properties through the constraints of the optimization (Asteasuain et al. 2004; Sundaram et al. 2005). Another very common approach is the minimization of a single scalar objective function which corresponds to a weighted sum of quadratic deviations between the observed and desired polymer properties values (Hanai et al. 2003). Additionally, the weighted sum is frequently used for multi-objective optimization with conflicting objectives such as batch time minimization and monomer conversion maximization or polydispersity minimization (Zhang 2004; Lemoine-Nava and Flores-Tlacuahauc 2006; Curteanu et al. 2006). Although this approach may be straightforward to implement, it requires the arbitrary definition of weighting factors which even for those familiar with the problem is not easy. In addition, slight variations in the weighting factors may yield a quite different solution, in such a manner that an optimal solution may be missed. Some attempts (Mitra et al. 2004; Agrawal et al. 2006; Konak et al. 2006) have also been made to obtain Pareto sets of candidate optimal solutions, which are sets of non-dominated solutions with respect to each other, i.e. while moving between two solutions, one objective function improves while the other worsens. The choice of the optimal solution in the Pareto set, however, requires not only process knowledge, but also some degree of arbitrariness and intuition.

Batch time or monomer conversion may be correlated with operational costs and incomes, but some trade-offs

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between process variables may not ensure the most efficient operation in economic terms if only time or conversion are considered as objective functions. On the other hand, an objective function considering only the deviations from the target properties may not lead to optimal operation from an economic point of view because several operational conditions may yield the same polymer grade. Bearing this as well as the above-mentioned drawbacks of multi-objective optimization in mind, a more robust approach should focus on operational profit as objective, while satisfying the desired polymer properties through the constraints of optimization.

The present work attempts to determine optimal operating strategies to target polymer resins for an industrial large-scale polymerization reactor, while seeking economic objectives, unlike the usual approach in literature as discussed. The polymer quality is ascertained through molecular properties that can be readily correlated to end-use properties, instead of solely considering average molecular weight and polydispersity. The molecular properties considered are melt index (MI), which measures the average molecular weight, and stress exponent (SE), related to the polydispersity of the molecular weight distribution (MWD). These properties can be correlated with polymer end-use properties such as stiffness, impact strength, elongation, tensile stress and melting temperature, for example (Costa et al. 2008), which are dictated by the final customers.

The problem is solved by genetic algorithm (GA), a powerful alternative for complex and highly non linear problems where the computation of derivatives becomes difficult. It does not require an initial estimate to find an optimum, as the deterministic methods, but it can still be improved if some problem knowledge is given to the initial population. Furthermore, there is a tendency but no guarantee that the GA will reach the global optimum. For these reasons, the GA has gained acceptance in almost all areas of science and engineering (Ghrayeb and Phojanamongkolkij 2005; Lombardi et al. 2006; Feng et al. 2014), and polymer reaction engineering is no exception (Kasat et al. 2003; Mitra et al. 2004; Zhang 2004; Lemoine-Nava and Flores-Tlacuahauc 2006; Curteanu et al. 2006; Agrawal et al. 2006; Ramteke and Gupta 2011). Despite of that some authors use GA to find an initial estimate for deterministic algorithms (Chakravarthy et al. 1997; Costa et al. 2005; Lombardi et al. 2006) due to its ability to search a broader space of candidate solutions whereas the second are very sensitive to the initial guess. Conversely, this paper proposes a hybridization approach showing that previous knowledge, which might come from process experience or previous optimization results, allows for a considerable improvement to the GA performance, i.e. optimum value and speed of convergence. This hybridization approach, therefore, might guide the GA towards near-global optimal solutions. The choice of the best set of GA parameters is usually ignored in literature. Here the design of experiments is used in order to investigate the main effects, as well as interaction effects, among the parameters and then define the best set.

The paper is structured as follows. Firstly, the industrial application of this proposal is discussed, followed by the optimization problem formulation and solution. Some results are discussed and an industrial example is illustrated. Finally conclusions are presented.

2 Process description

The case study investigated is an industrial scale polymerization process, depicted in Figure 1, which produces high density polyethylene (HDPE). Two reactors are connected in series: a non-ideal CSTR (Continuous Stirred Tank Reactor) and a PFR (Plug Flow Reactor). A mixture of catalyst (CAT) and co-catalyst (CC), monomer (M), hydrogen (H_2) and solvent (S) is continuously fed to reactor. The main feed (W_t) is split between the top (side feed, W_s) and the bottom of the reactor in order to enhance mixing inside the reactor. The mathematical model of the process has been developed and validated in previous studies (Embiruçu et al. 2000; Pontes et al. 2010) and the kinetic and physical parameters have been exhaustively validated with actual dynamic data (Embiruçu et al. 2008). Depending on the operating condition, i.e. reactants feed concentrations, flow rates and temperature profiles, several grades of HDPE might be produced. In industrial practice, therefore, there is a so-called synthesis condition which dictates the operating conditions of each grade to be produced. Such synthesis conditions are based on engineers and operators knowledge. When designing new grades, usually production scale experiments are carried out based on indeed empirical correlations between inlet and outlet variables, the so-called “short-cut calculations”. This leads to a time-delayed trial and error procedure which might produce off-spec material that is usually discharged or sold by a lower price.

On the other hand, current market competition demands high quality products and just in time production to satisfy costumers needs. Optimization tools are then required for those who want to excel in this scenario. A software able to dictate optimal operating condition to target polymer resins while seeking economic

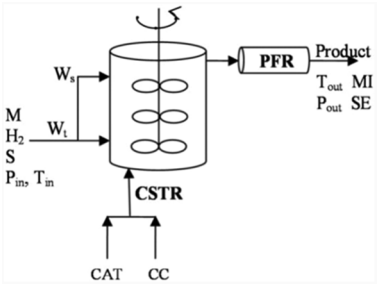

Figure 1: Schematic diagram of the industrial polyethylene reactor.

objectives might then afford great opportunities for the process operation. Such an optimization model might be used in different time-scales: at low-frequency to dictate optimal synthesis conditions for new or existing polymer grades; or at high-frequency to give set-points to underlying controllers in on-line optimization architectures.

3 Optimization problem

3.1 Problem formulation

Based on previous process analysis (Pontes et al. 2011), the degrees of freedom of the optimization are:

$$\mathbf{u} = [\,\mathrm{M} \quad \mathrm{H_2} \quad \mathrm{CAT} \quad \mathrm{W_t} \quad \mathrm{W_s} \quad \mathrm{P_{in}}\,]^{\mathrm{T}} \tag{1}$$

where P_{in} is inlet pressure. Variables in eq. (1) must be kept within limits in order to avoid operational problems, such as pump cavitations due to a high hydrogen inlet concentration or phase separation due to low inlet pressure.

Polymer quality in this industrial process is verified at the outlet of the PFR, i.e. at the end of the reaction, through the melt index and stress exponent. In order to target these properties, the desired values should be satisfied through constraints on the optimization problem. Hence, a vector of constraints, either equality or inequality, at the PFR outlet may be defined as:

$$\mathbf{h} = [\,\mathrm{MI} \quad \mathrm{SE} \quad \mathrm{T_{out}} \quad \mathrm{P_{out}}\,]^{\mathrm{T}} \tag{2}$$

where T_{out} and P_{out} are outlet temperature and pressure, additionally constrained to ensure safe operation. The MI is a measure of the polymer average molecular weight: the higher the MI, the lower the molecular weight. On the other hand, SE is a measurement of the polydispersity of the MWD: a broader MWD or higher polydispersity corresponds to a higher SE value. Polymer density could additionally be included as a target property, but it is greatly influenced by comonomer content. As the present study focuses on the homopolymerization process, MI and SE are mainly used to specify the polymer quality.

As previously mentioned, in order to obtain more reliable results, the optimization should consider economic aspects in the objective function, which is then given by:

$$\begin{aligned}\Phi \;=\; & a \cdot W_{PE} - \left(b_M \cdot W_M + b_H \cdot W_H + b_{CAT} \cdot W_{CAT}\right. \\ & \left. + b_{CC} \cdot W_{CC} + b_S \cdot W_S\right) \text{€/s}\end{aligned} \tag{3}$$

where a is the polyethylene sales price (€/kg), b_j represents the cost (€/kg) of raw material j, W represents mass flow rates and the subscripts PE, M, H, CAT, CC and S denote polyethylene, monomer, hydrogen, catalyst, co-catalyst and solvent, respectively. Part of the solvent is recycled to reactor after separation processes, which are not included in the model, so that it is not possible to compute the flowrate of the solvent makeup stream. Therefore, the total inlet flowrate of the solvent is considered in the profit function. Energy and losses could be considered in a more comprehensive and complete objective function. However, the system is adiabatic and possible energy losses due to non-ideal insulation are not easily measured and may be neglected. Moreover, the inlet temperature is much lower than the reaction temperature with the result that energy consumption through heating reactants can also be neglected.

The optimization problem is then formulated according to:

$$\max_{\mathbf{u}} \Phi \tag{4}$$

s.t.

$$\mathbf{x} = \mathbf{f}(\dot{\mathbf{x}}, \mathbf{y}, \mathbf{u}, \mathbf{p}, z), \tag{4a}$$

$$0 = \mathbf{g}(\dot{\mathbf{x}}, \mathbf{y}, \mathbf{u}, \mathbf{p}, z), \; z \in [z_0 z_f], \tag{4b}$$

$$\mathbf{J}(\dot{\mathbf{x}}_1, \mathbf{x}_1, \mathbf{y}_1, \mathbf{u}_1, \dot{\mathbf{x}}_0, \mathbf{x}_0, \mathbf{y}_0, \mathbf{u}_0, \mathbf{p}, z) = 0, \tag{4c}$$

$$\mathbf{u}_{LB} \le \mathbf{u} \le \mathbf{u}_{UB}, z = z_f, \tag{4d}$$

$$\mathbf{h}_{LB} \le \mathbf{h} \le \mathbf{h}_{UB}, z = z_f, \tag{4e}$$

where eq. (4a) represents the PFR mass and energy balances, eq. (4b) summarizes the algebraic equations that represent the CSTR and additional correlations for output process variables such as conversion, polymer production rate and polymer properties, eq. (4c) maps the CSTR outlet to the PFR contour condition, $\mathbf{x}$ are differential state variables, $\mathbf{y}$ the algebraic state variables, $\mathbf{u}$ the control variables, $\mathbf{p}$ the invariant parameters, z the axial coordinate. Subscripts 0, 1 and f refer to CSTR inlet, PFR inlet and PFR outlet respectively, and LB and UB are the lower and upper bounds for the decision variables ($\mathbf{u}$) and constraints ($\mathbf{h}$).

3.2 Solution based on genetic algorithm

Optimization is carried out by the genetic algorithm (GA), a stochastic method that mimics the mechanism of natural selection, i.e. the fittest individuals survive in a competitive environment. Basically, three operators are responsible for the GA search potential: reproduction, crossover and mutation. In the current approach reproduction is based on tournament selection, which randomly picks out two individuals, compares them, and selects the fittest one for the next generation. Since offsprings replace parents in a population, the best solution can die out. In order to ensure that the fittest individual from a generation will propagate to the next one, an elitism operator is used.

Each individual or chromosome has to be coded, e.g. into binary or real representation. If real codification is adopted, proper crossover and mutation operators have to be used (Silva and Biscaia 2003; Curteanu et al. 2006; Deb and Goyal 1996). The simulated binary crossover (SBX) and the parameter based mutation, as suggested by Deb and Goyal (1996), are applied here for the real codification. This operators maintain the interval schema processing and are then supposed to match the search power of the binary operators.

The optimization problem addressed here requires some equality and inequality constraints, as eq. (4) states. A frequently used technique to handle constraints is to introduce a penalty function to the objective function. However, a problem that arises when using this approach is the definition of penalty parameters. Silva and Biscaia (2003) adopt a fuzzy penalty function method to transform constrained multi-objective optimization problems into non-constrained ones. Deb (2000) proposes a constraint handling method based on the tournament selection potential that does not require the definition of penalty parameters, therefore this approach is applied here. For the selection of the best individual, the following criteria are used: (a) when two feasible solutions are compared, the one with the best objective function is selected; (b) when a feasible solution is compared with an unfeasible solution, the former is selected; (c) when two infeasible solutions are compared, the one that less violates the constraint is adopted.

The genetic algorithm was implemented in Fortran code and combines features from the codes published by Deb (2001) and Carroll (2001). The time required for the optimization is given by $t_{exe} = t_0 \cdot N_p \cdot N_g$, where t_0 is the time in seconds required for a single process simulation, N_p is the population size and N_g is the number of generations, here chosen as termination criterion. A single process simulation takes around 1 s on an Intel Core 2 Quad 2.39 GHz. Therefore, a typical optimization with $N_g = 100$ and $N_p = 100$ takes around 2.8 h to run.

3.2.1 GA parameters tuning

In order to use the GA, a number of parameters have to be set. The present study includes crossover and mutation probability (p_c and p_m, respectively), population size (N_p), chromosome length (l), when using binary codification, and a seed number for random initial population generation (*seed*). It is important to note that for a specific seed number the same initial population is generated every time the code is run. The studies in literature concerning the GA do not usually mention the reason why the set of parameters used in optimization was chosen. On the other hand, Silva and Biscaia (2003) and Zhou et al. (2000) perform one-factor-at-a-time experimentation in order to evaluate the effects of some GA parameters on optimization performance. However, this approach fails to identify and to quantify the interaction effects among parameters. Costa et al. (2005, 2007) propose a systematic procedure to determine the best set of GA parameters based on design of experiments, as also suggested by Ghrayeb and Phojanamongkolkij (2005). This technique evaluates several GA parameters at the same time in order to determine which factors and interaction between variables really exert a significant effect on the final response.

The present study carries out an experimental design for each codification scheme in order to identify the best GA parameters set. For the real codification, a 2^4 full factorial design is carried out, making up a total of 17 runs, including a central point. However, if a complete design were carried out for the binary codification, the number of trials would rise to 33. The computational time mentioned above encourages therefore a $2v^{5-1}$ fraction factorial design for binary codification. One trial at the central point is carried out as it provides an additional degree of freedom for estimating the effect's standard deviation, which is important when testing the significance of effects (Burkert et al. 2004). The design matrixes are shown in Table 1 for real and binary codification, where Φ is the best objective function within 100 generations. Normalized values are used due to confidentiality reasons.

Using real codification, trials 15 and 16 did not find a feasible solution within 100 generations, therefore a very low objective value is assigned. On the other hand, all the trials using binary codification were found to be feasible.

Table 1: Design matrix.

Real codification: 2^4						Binary codification: $2v^{5-1}$					
Trial	*seed*[1]	p_m[2]	p_c[3]	N_p[4]	Φ (dim.)	*seed*	p_m	p_c	l[5]	N_p	Φ (dim.)
1	+1	+1	+1	+1	71.58	+1	+1	+1	+1	+1	88.91
2	−1	+1	+1	+1	42.58	−1	+1	+1	+1	−1	87.80
3	+1	−1	+1	+1	68.92	+1	−1	+1	+1	−1	88.78
4	−1	−1	+1	+1	88.82	−1	−1	+1	+1	+1	87.42
5	+1	+1	−1	+1	62.37	+1	+1	−1	+1	−1	87.69
6	−1	+1	−1	+1	**89.54**	−1	+1	−1	+1	+1	87.55
7	+1	−1	−1	+1	42.67	+1	−1	−1	+1	+1	88.10
8	−1	−1	−1	+1	62.98	−1	−1	−1	+1	−1	85.53
9	+1	+1	+1	−1	79.54	+1	+1	+1	−1	−1	88.86
10	−1	+1	+1	−1	89.29	−1	+1	+1	−1	+1	89.33
11	+1	−1	+1	−1	64.85	+1	−1	+1	−1	+1	86.80
12	−1	−1	+1	−1	73.22	−1	−1	+1	−1	−1	64.65
13	+1	+1	−1	−1	60.42	+1	+1	−1	−1	+1	**89.68**
14	−1	+1	−1	−1	71.28	−1	+1	−1	−1	−1	87.14
15	+1	−1	−1	−1	0.00	+1	−1	−1	−1	−1	89.52
16	−1	−1	−1	−1	0.00	−1	−1	−1	−1	+1	50.52
17	0	0	0	0	58.20	0	0	0	0	0	89.49

Note: Levels −1, 0, +1: 0.10, 0.25, 0.40[1]; 0.01, 0.03, 0.05[2]; 0.7, 0.8, 0.9[3]; 80, 90, 100[4]; 8, 9, 10[5].

The best objective values are 89.54 (from trial 6) and 89.68 (from trial 13) for the real and binary codifications, respectively. Despite the slight difference of 0.03% based on the non-normalized Φ values, it is possible to observe from Table 1 that binary codification yields the best overall performance.

The software package Statistica (Statsoft, v. 6.0) was used to analyze the results. The Pareto sets in Figure 2 for both codifications show the standardized effects, i.e. the effects divided by their respective standard errors. The vertical lines (p = 0.05; p = 0.10) indicate the minimum magnitude of statistically significant effects, considering the statistical significance of 95% or 90%. Therefore an analysis of the Pareto charts enables the identification of the statistically significant effects as well as the most relevant factors. For real codification, mutation and crossover probability as well as their interaction effects with each other and with population size present statistically significant effects. Therefore the use of higher crossover and mutation probabilities alone is inefficient to achieve a better optimum. The results in Table 1 corroborate this observation and therefore the optimal parameter set chosen is that identified in trial 6, which yields the best optimum: seed = 0.1, p_m = 0.05, p_c = 0.07, N_p = 100.

Unlike real codification, no parameter has statistically significant effect using binary codification. This observation is not surprising since different mutation and crossover operators are used. Comparing the results in Table 1, it is possible to attribute the variation in the Φ values in the binary codification to a noise inherent to the random characteristic of GA. Hence, the optimal parameter set is chosen to be: seed = 0.4, p_m = 0.05, p_c = 0.07, l = 8; N_p = 100; i.e. the set from trial 13. As mentioned earlier, Zhou et al. (2000) evaluate the parameters of a binary

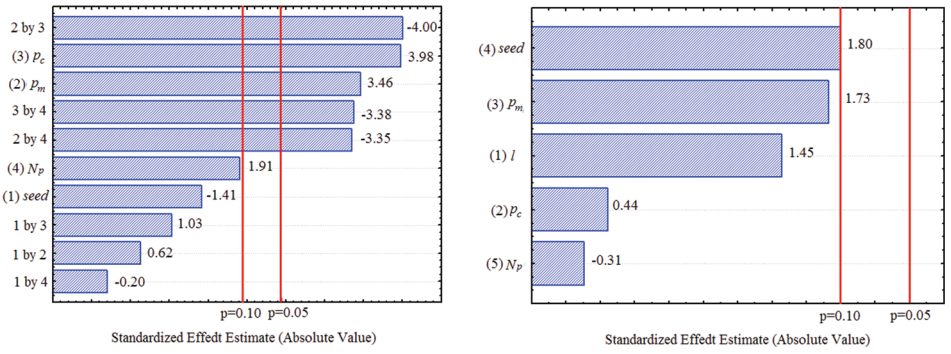

Figure 2: Pareto charts for real (left) and binary (right) codifications.

coded GA, while Silva and Biscaia (2003) study a real coded GA. These studies did not find significant changes when varying parameters such as population size and crossover and mutation probability. The designs of experiments carried out here are in accordance with Beasley *et al.*'s (Beasley et al. 1993) findings. They observe that the basic mechanism of GA is so robust that parameter setting is not crucial, but the fitness function and the coding scheme used are indeed critical in the performance of a GA. Ghrayeb and Phojanamongkolkij (2005), which also employed the design of experiments to select the GA parameters, come to inconclusive results, mentioning that there is no guideline in setting GA parameters to obtain the best optimal solution.

3.3 Hybrid approaches

Many authors report problems when using deterministic optimization methods for highly non-linear models, proposing hybrid methods where the GA gives the initial estimate for the deterministic algorithm (Chakravarthy et al. 1997; Costa et al. 2005; Lombardi et al. 2006). On the other hand, there are some hybrid approaches for the GA that often outperforms the conventional method, as the incorporation of heuristics into initialization to generate well-adapted initial population. If elitism operator is further considered, then, the hybrid GA cannot be worse than the conventional GA. The present study, therefore, proposes to incorporate special individuals into the GA initial population in order to guide the search for the global optimum.

Since the process investigated is an industrial scale reactor, some operating conditions might be known from practice. Therefore, some arbitrary operating condition might be included into the GA random initial population, approach that is called here GA-I. As mentioned above, in industrial practice there is a synthesis condition for each grade produced. If the current operating condition for the respective grade is the initial guess, the approach is called GA-II. Therefore, the latter contains more knowledge than the former. If new grades are target, i.e. if a synthesis condition is not known in advance, a sequence of n optimizations may be carried out so that previous runs with the GA itself may supply the initial guess, guiding the search. The sequential method (GA-SQ), then, carries out n sequential optimizations using information from the optimum from the $(n-1)$th iteration, and no additional information is necessary. Therefore, conversely to the approaches in literature, these hybridization schemes exploit the availability of previous results or process experience to improve GA performance without necessarily combining it with a deterministic approach.

4 Results and discussion

Several optimization studies were carried out in order to target a broad range of polymer grades. Firstly, two sequences of optimizations were carried out: 1) varying MI with a constant SE = 0.255 ± 0.005; 2) varying SE with a constant MI = 0.288 ± 0.006. Secondly, the hybridization approaches GA-I and GA-SQ are tested in order to verify and compare their potential of improving the optimum result. In all optimizations the same bounds for outlet temperature and outlet pressure (T_{out}, P_{out}) were used. Last but not least, the synthesis conditions of two commercial polymer grades are optimized (GA-II). All results are normalized, therefore dimensionless (-), due to confidentiality reasons.

Figure 3 illustrates the profit function, and Figure 4 the decision variables profiles. For the sake of clarity, some profiles for Example 1 are omitted. The side feed and the catalyst concentration present the most

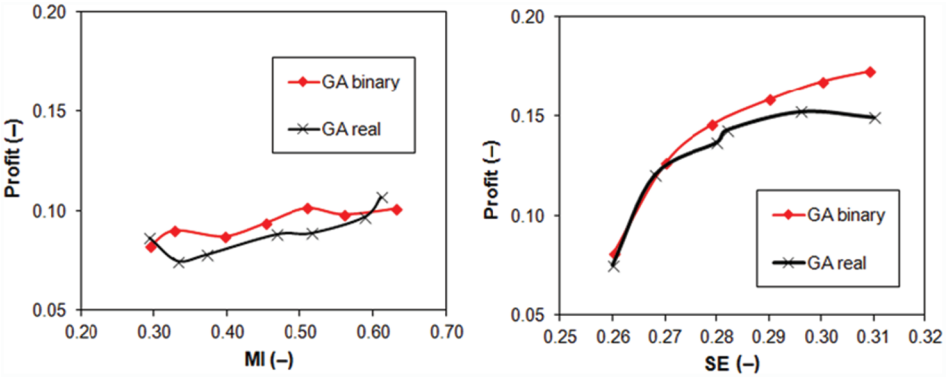

Figure 3: Profit *versus* MI and SE: Left, Example 1 (SE = 0.255 ± 0.005); Right, Example 2 (MI = 0.288 ± 0.006).

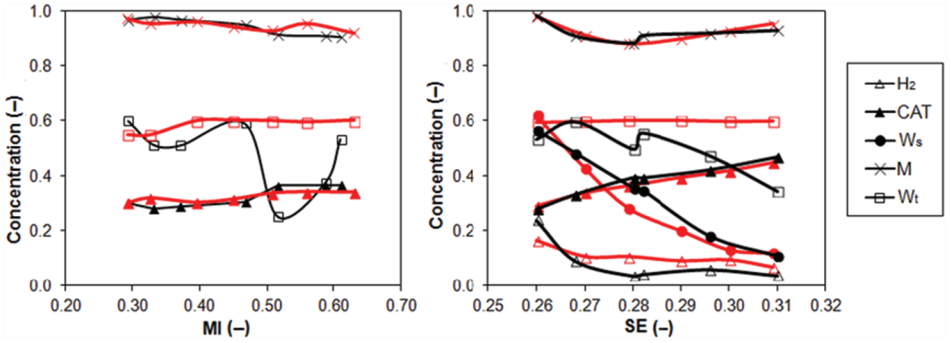

Figure 4: Decision variables *versus* MI (Example 1: SE = 0.255 ± 0.005) and SE (Example 2: MI = 0.288 ± 0.006): Red, GA binary; Black, GA real.

meaningful changes on SE, as the slopes in Figure 4 suggest. Catalyst and monomer concentrations have the greatest effect on profit because of their higher raw material costs in eq. (3). Therefore, despite the increasing catalyst concentration, the lower or nearly constant monomer consumption ensures higher profits. This observation supports the importance of maximizing profit instead of minimizing deviations from targets or production time, as usually approached in literature. A detailed description of the physicochemical phenomena taking place inside the reactor has been presented in previous works (Pontes et al. 2008, 2010).

The binary codification shows better results than the real codification since the latter reproduces the random characteristic of the method mainly at the main feed (W_t) profile, which has a great impact on profit. Given that a phenomenological model represents the process, it seems that GA failed to locate the global optimum for some optimizations. According to Rangaiah (2001), GA is very good at identifying promising regions where the global optimum lies, but it is poor at determining the optimum point with accuracy. It indicates therefore that the results might be in the vicinity of the global optima.

As discussed before, two hybridization methods are proposed in order to improve GA performance. The first one introduces knowledge from the industrial practice into the initial population: an arbitrary operating condition (GA-I) or the synthesis condition for the respective polymer grade (GA-II). The second one (GA-SQ) carries out a sequence of optimizations so that the result from the previous run is the initial guess to the next optimization.

In order to evaluate the hybridization methods, the grade SE = 0.310 and MI = 0.288 from Example 2 is taken for analysis due to its poorer results for real encoding. Since there is no synthesis condition for this grade, an arbitrary operating condition is given to the initial population, therefore scheme GA-I is used. The results for the objective and penalty functions over generations are summarized in Figure 5. Although the initial guess is a non feasible solution, it allows the GA-I real to find the feasible region sooner so that it has a faster convergence and gets to a profit 13.22% higher than the GA real and just 1.9% lower than GA binary. The hybridization allowed for a considerable improvement in GA, not only due to the better optimum, but also due to the faster convergence, indicating that GA might have found the global optimum. Therefore, a random initial population which does not contain a sufficient number of individuals near the feasible space may inhibit a satisfactory search for an optimum by the real GA method, what may be overcame by using binary encoding or the hybridization approach suggested.

Figure 6 illustrates the results of the GA-SQ, when evaluating the sequence of Example 1. The vertical

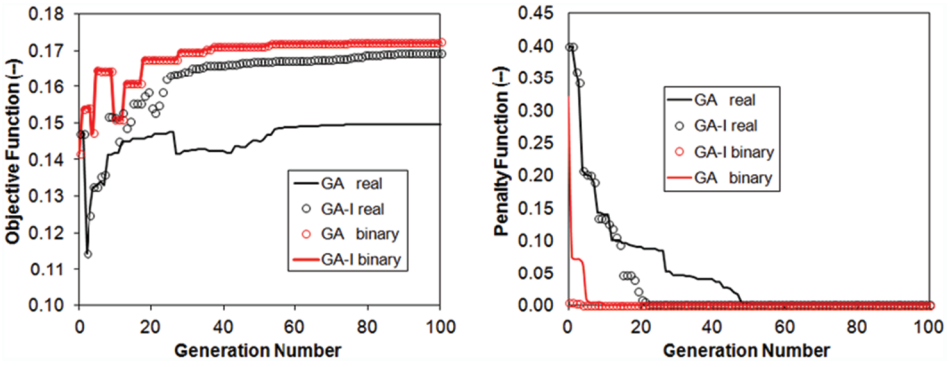

Figure 5: Hybridization approach GA-I for SE = 0.310 and MI = 0.288.

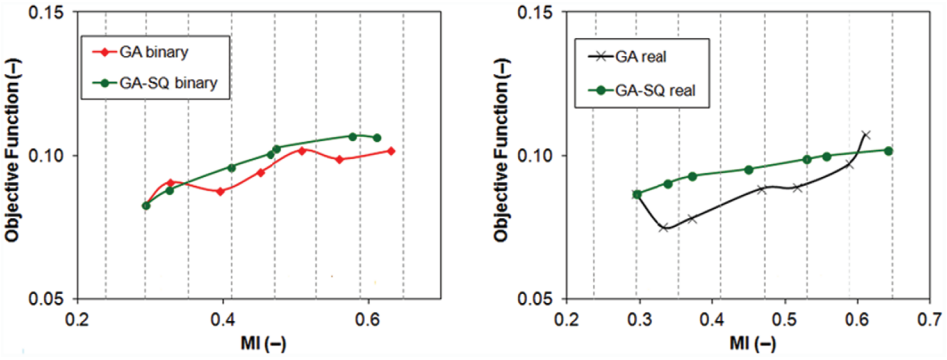

Figure 6: Example 1 – comparison between GA and GA-SQ for binary (left) and real (right) codifications.

dashed lines represent lower and upper bounds for MI, i.e. the specification limits for the target polymer. There is a significant improvement on the GA performance since both codifications found overall higher profits. The sequential optimization allowed GA to find a feasible space at the very beginning, around the third and seventh generation, what affords its application even for online purposes.

The optimization problem formulated is useful not only to design new polymer grades but also to optimize current operating conditions. Two commercial polymer grades, R-01 (MI = 13.435 ± 0.071; SE = 0.260 ± 0.900) and R-02 (MI = 2.341 ± 0.071; SE = 0.270 ± 0.900), are taken for optimization. As mentioned above, for each grade there is a synthesis condition which might be given as initial guess to the GA random initial population, so that the GA-II can be employed. Table 2 illustrates the increase in profit with regard to the value computed at the synthesis condition. The optimization allows significant improvements which can reach up to 25% higher profit. Binary GA-II outperforms, result that is in accordance with the previous findings. The higher profits are associated with a greater polymer production rate (W_{PE}). If the market cannot afford such throughput, it might be constrained by the value computed at the synthesis condition, what is further illustrated in Table 2. Even though, profits 3% higher might be obtained by the optimization.

Table 2: Comparison of different GA approaches when optimizing synthesis conditions.

	GA real (%)	GA-II real (%)	GA binary (%)	GA-II binary (%)	GA-II binary W_{PE} constrained (%)
R-01	15.64	18.20	18.86	24.36	3.16
R-02	9.19	5.82	15.18	19.95	3.37

5 Conclusion

This paper presents an optimization problem for the design of tailored polymer resins while considering economic objectives using GA. When optimizing known synthesis conditions, profits up to 25% higher than the industrial practice were achieved. That indicates the great potential of the optimization problem here formulated. Since the availability of a robust deterministic algorithm is not common, GA presents itself as a potential alternative. It might be used online at different time-scales: at low-frequency to dictate optimal synthesis conditions for new or existing polymer grades; or at high-frequency to give set-points to underlying controllers in on-line optimization architectures.

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