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Non-dominated Sorting Genetic Algorithm Used for Optimization of the Siloxane-Siloxane Copolymers Synthesis

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Abstract

This paper presents a software implementation of the elitist non-dominated sorting genetic algorithm (NSGA-II) applied to the optimization of a complex polymerization process. A neural network modeling the variation in time of the main parameters of the process was used to calculate the vectorial objective function included in the NSGA-II. The algorithm provides the optimum decision variables (reaction temperature, concentration of the catalyst, reaction time, and initial composition) which maximize the reaction conversion and minimize the difference between the obtained copolymer composition and the desired copolymer composition. The algorithm has proven to be able to find the entire non-dominated Pareto front and to quickly evolve optimal solutions as an acceptable compromise between objectives competing with each other.

Key words: *neural network, non-dominated elitist sorting genetic algorithm, optimization, siloxane copolymer.*

Introduction

The optimization of a polymerization process is multi-objective in nature, since it has several objectives, often non-commensurable and competing with each other, that must be satisfied at the same time. Therefore, solving such a problem is accompanied by difficulties starting with the way of formulating the objective function and continuing with the choice of working procedure and selection of the results from more possible options. In the last several years, some research has been reported in the literature on the optimization of polymerization reactors using multiple objective functions and constraints.

Many optimization techniques involved single (scalar) objective function which incorporates several objectives and uses a *weighted average combination* [1]. This approach was applied to a complex polymerization process in one of our previous studies [2]. The optimization method was found to be simple to use, but depending on the user's decision to specify weights to the different objectives based on good knowledge of the process. This can be a drawback when the objectives to interrelate are of different nature. A simple genetic algorithm has been used to generate optimal weights and eliminate the user's implication at this step of the optimization process, but the risk of losing some optimal solutions remained.

A much better approach was reported to be the multi-objective optimization with *objective functions that are vectors* [3]. As all the objectives are simultaneously treated, multi-objective

optimization problems lead to a set of non-dominated solutions, known as *Pareto optimal solutions*, as opposed to the single solution provided by any single objective optimization task. Although only one solution must be chosen at the end of the optimization exercise and this often must be performed with the guidance of a decision-maker, it is a better practice to first find a set of Pareto optimal solutions to have an idea of the extent of possible trade-offs among the underlying objectives before focusing on a particular solution [4].

Extensive research has been reported in recent literature on the algorithms used for generating non-dominated Pareto optimal solutions. Evolutionary algorithms (EA) have been recognized to be particularly suitable to solve multi-objective optimization problems because they simultaneously deal with a set of possible solutions which allows an entire set of Pareto optimal solutions to be evolved in a single run of the algorithm, instead of having to perform a series of separate runs as in the case of traditional mathematical programming techniques [5]. Thus, many evolutionary multi-objective optimization algorithms were developed among which Non - dominated Sorting Genetic Algorithm (NSGA and its enhanced version NSGA-II) has been found effective in solving a wide variety of problems. Multi-objective optimization of the polymerization processes is an example of their applications [6].

This paper proposes a software implementation of NSGA-II applied to the optimization of a complex polymerization process – synthesis of dimethyl-methylvinylsiloxane copolymers. The reactions for polysiloxane synthesis are very complex, with many reactions concomitantly occurring. The variation in time of the main parameters of the process (conversion and copolymer composition) was modeled with a feed-forward neural network which computes the fitness functions used by the genetic algorithm. The conflicting objectives were the maximization of the reaction conversion and the achievement of a desired value for copolymer composition. The decision variables optimized with NSGA-II were reaction conditions: temperature, concentration of the catalyst, reaction time, and initial composition.

Multi-Objective Optimization Method

The reactions for polysiloxane synthesis are very complex, a series of ring-opening polymerization, polycondensation, depolymerization by cyclization and chain scrambling reactions occurring in the same time, except for the case when the conditions for the kinetical control are created. It is of high interest to know the conditions in which copolymers with desired compositions in maximum yields can be obtained. Thus, the multi-objective optimization problem consists in maximizing the reaction conversion and achieving a desired value for copolymer composition, the decision variables being the reaction time, the temperature of the copolymerization process, the amount of catalyst, and the initial composition of the reaction mixture.

The multi-objective vectorial function is composed of two fitness functions:

$$f = (x, -(F1 - F1d)^2) \tag{1}$$

and the bounds for the decision variables are:

$$0 \le F1 \le 1, \quad 0 \le x \le 100, \quad 20 \le T \le 110, \quad 0.25 \le t \le 2.25, \quad 0.5 \le C \le 5, \quad 0 \le f1 \le 1, \tag{2}$$

where x is the reaction conversion, $F1$ is the copolymer composition, $F1d$ is the desired copolymer composition, t – the reaction time, T – temperature of the copolymerization process, C – amount of catalyst, $f1$ – initial composition of the reaction mixture.

The parameters x and $F1$ are computed using a neural network (NN) which models the variation in time of the main parameters of the process (conversion and copolymer composition), which can be represented as:

$$\text{NN [Inputs: t, T, C, f1; Outputs: x, F1]} \ . \tag{3}$$

NSGA-II is the elitist non-dominated sorting genetic algorithm used to obtain the optimum decision variables which maximize the reaction conversion and minimize the difference between the obtained copolymer composition and the desired copolymer composition.

The algorithm uses chromosomes (solutions) with 4 real-coded genes, tournament selection for the parents of a new chromosome, arithmetic crossover (the generation of a random number between 0 and 1 representing the fraction of information taken from the mother chromosome, the rest being taken from the father chromosome) and mutation through resetting (the generation of a random value between the minimum and the maximum real values of the gene). The steps describing the working principle of the proposed software implementation for NSGA-II, as adapted for the studied optimization problem, are presented next:

1. Load parameters of the problem: popSize, noGen, F1d, TournamentSize, CrossoverProbability, MutationProbability.
2. Initialize the population of chromosomes with real random values in the specified bounds. Compute the fitness for every chromosome using NN model. Number of generations = 0.
3. Sort the population of chromosomes using non-dominated Pareto fronts according to the fitness. Assign crowding distance to every chromosome based on a ranking matrix constructed from the partial fitness of every chromosome.
4. Obtain popSize child chromosomes by selecting parents based on rank and crowding distance and applying crossover and mutation. Create a new temporary population of size 2*popSize formed half from chromosomes representing the parents' generation and half from chromosomes representing the children generation. Execute step **3.**
5. Select a new population of popSize chromosomes based on Pareto dominance and crowding distance. Number of generations increases with 1.
6. If the number of generations is lower than noGen, then go to step 4, else go to step 7.
7. Get the solution vector - the non-dominated Pareto front.
8. Calculate F1 and x using NN model.
9. Print the solutions: the optimum decision variables and the corresponding copolymer conversion (x) and composition (F1).

In the pseudocode presented above, *popSize* represents the number of chromosomes in a population and *noGen* is the maximum number of generations.

In order to define Pareto dominance, we say that a chromosome dominates another chromosome if all its partial fitness functions are greater than or equal to those of the other chromosome and one is strictly greater.

A non-dominated Pareto front is a set of Pareto non-dominated solutions.

The neural network used for modeling the conversion and copolymer composition is a multilayer perceptron, a feed-forward neural network trained with back-propagation algorithm. A configuration of 4 input neurons, a single hidden layer with 10 neurons, and an output layer with 2 neurons, noted MLP(4:10:2), was used.

Results and Discussion

A series of simulation were performed using different parameters for the NSGA-II. Various values for population size (50, 100, 200, 500) and number of generations (100, 200, 500, 1000,

2000) were tested with the values for the crossover probability and the mutation probability set to 0.9 and 0.03, respectively. The results of the simulations showed that better fitness functions are obtained when the population size increases, but only to a certain point. Beyond that, a larger population decreases the convergence speed of the algorithm, without leading to an improvement of the solution. With the increase in the number of generations, the execution time increases, but the use of elitism guarantees the fact that the solution will not worsen over time. The best results were obtained for a population size of 50 individuals and 500 generations.

With the population size set at 50 and the number of generations set at 500, the simulations were continued using different values for the crossover probability (0.9 to 0.1) and the mutation probability (0.01 to 0.8). It has been observed that better fitness function values were obtained for a crossover probability between 0.7 and 0.9. The best results were obtained for a crossover probability of 0.9 and a mutation probability of 0.1. Table 1 presents some solutions – the most appropriate for the polymerization process discussed – selected from the Pareto fronts obtained after the simulations with different values for the NSGA-II parameters.

Table 1. Selected results from the Pareto fronts

No.	NSGA-II parameters				Decision variables				Fitness functions	
	Pop size	No Gen	Crossover Probability	Mutation Probability	t	T	C	f1	x	F1
1	50	500	0.9	0.03	2.155	94.807	4.704	0.613	70.260	0.724
2	50	1000	0.9	0.03	1.114	87.445	4.318	0.693	65.216	0.717
3	100	100	0.9	0.03	1.346	105.051	4.922	0.931	70.882	0.742
4	200	500	0.9	0.03	1.517	101.570	4.785	0.919	71.095	0.763
5	50	500	0.8	0.03	1.604	82.881	4.265	0.717	69.089	0.754
6	50	500	0.5	0.03	0.875	106.287	4.780	0.856	68.085	0.757
7	50	500	0.9	0.01	1.382	104.083	2.554	0.823	66.945	0.709
8	50	500	0.9	0.1	1.929	101.251	4.130	0.637	70.481	0.711
9	50	500	0.9	0.5	1.725	106.249	3.650	0.817	70.724	0.731
10	50	500	0.9	0.8	1.422	86.070	4.600	0.717	68.387	0.711

Considering the results in Table 1, the appropriate parameters of GA used to solve the proposed optimization problem are: popSize = 50, noGen = 500, crossover_probability = 0.9 and mutation_ probability = 0.1.

The non-dominated Pareto front obtained using the parameters mentioned above is illustrated in figure 1. By comparing the solutions in the Pareto front, it can be noticed that each of them optimizes an objective to the detriment of the other. A solution can be chosen only by considering an objective more important than the other, as a function of the user's desire and goal.

The results presented in Table 1 were chosen by considering the achievement of a desired value for copolymer composition more important than a maximum reaction conversion. The imposed value for the copolymer composition was F1d = 0.7.

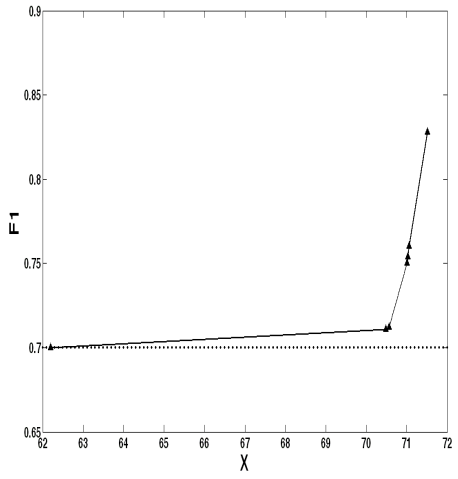

Fig. 1. Pareto optimal set.

By analyzing the results of the simulations, it can be observed that F1 has values closed to F1d, but the reaction conversion, x, is relatively small. In the case of the dimethyl-methylvinylsiloxane copolymers, the relatively low values for conversion can be explained by the reversibility of the process. The position of the equilibrium depends on some factors, among which we can also mention the silicon substituent nature. Thus, by increasing the bulk of the substituents, the equilibrium shifts to the left and, as a result, the conversion will be lower. The experimental data showed in Table 1 reflect such situation: the maximum conversion does not exceed 72% irrespective of the combination of the parameter values being used.

Figures 2 and 3 illustrate the influence of the decision variables on the copolymer composition (F1) and the reaction conversion (x).

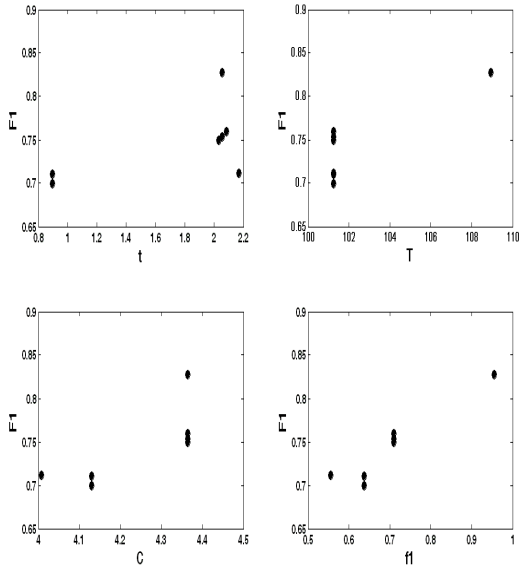

Fig. 2. Dependence of F1 on decision variables.

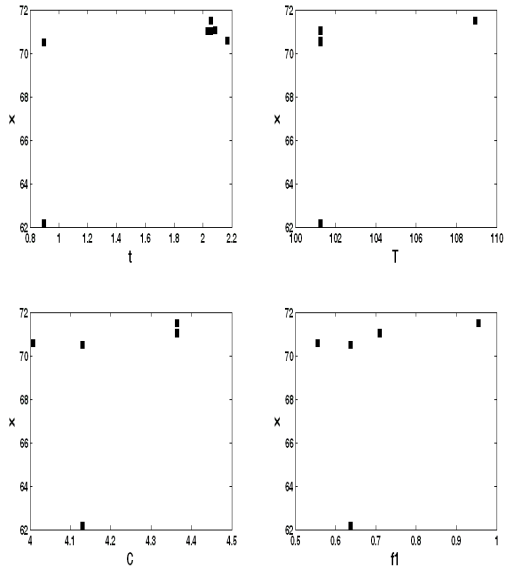

Fig. 3. Dependence of x on decision variables.

The optimization procedure is implemented in the C# programming language, and specific functions are programmed for each phase of the non-dominated sorting genetic algorithm (NSGA-II).

Conclusions

The multi-objective optimization problems of a polymerization process were approached with techniques involving scalar objective function representing the weighted average of several objectives. A much better approach was reported to be the multi-objective optimization with vectorial objective functions which lead to a set of non-dominated Pareto optimal solutions.

This study proposes a software implementation of NSGA-II adapted to the optimization of a complex polymerization process. A neural network modeling the variation in time of the main parameters of the process was used to calculate the fitness functions included in the NSGA-II.

The efficiency of the proposed method in finding the entire non-dominated Pareto front is illustrated by the obtained results which show that the algorithm can quickly evolve optimal solutions as an acceptable compromise between objectives competing with each other. Although the proposed method has been applied for an optimization problem with only two objective functions, it can also be directly used for problems with more than two objective functions and other processes for which the amount of knowledge is limited.

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Algoritm genetic de sortare nedominată aplicat în optimizarea sintezei copolimerilor siloxanici

Rezumat

Această lucrare prezintă o implementare software a algoritmului genetic de sortare nedominată (NSGA-II) aplicat optimizării unui proces de polimerizare complex. Funcţia obiectiv vectorială inclusă în NSGA-II a fost calculată cu o reţea neuronală ce modelează variaţia în timp a principalilor parametri ai procesului. Algoritmul a fost utilizat pentru a obţine variabilele de control optime care să maximizeze conversia reacţiei şi să minimizeze diferenţa dintre compoziţia finală a copolimerului şi cea dorită. Algoritmul s-a dovedit a fi foarte potrivit pentru obţinerea rapidă a întregului front Pareto, ce implică o serie de compromisuri între obiective divergente.