Investigation on Evolutionary Control and Optimization of Chemical Reactor

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Abstract. This contribution deals with a new algorithm – the Self-Organizing Migrating Algorithm (SOMA). The SOMA algorithm was used for static optimization of a given chemical reactor with 5 inputs and 5 outputs. SOMA was used on this reactor for static optimization because the reactor, which was set by an expert, shows poor performance behaviour. Participation consists of simulation results, which shows how expertly set reactor behaves. Also set of static optimization simulations of given reactor is presented here including results and conclusions.

Keywords: SOMA, migration, self-organization, evolutionary algorithms, global optimization, non-linear optimization, mixed discrete variables, penalty function.

1 Introduction

Nowadays, there exist a broad class of algorithms that can be, and are, used for optimization. This special class of algorithms is made up of so-called evolutionary algorithms (EA) similar to genetic algorithms or differential evolution algorithms [1]. Both algorithms work with so-called populations that are evolved in “generations” (or “Migration Loops” in the case of SOMA [2], [3], [4], [5], [1]), in which only the best-suited individuals survive.

This contribution presents a new algorithm, which can be labelled an "evolutionary" algorithm - despite the fact that during its activity, no new generations are created (in a general sense). Development of this algorithm was inspired by the behaviour patterns of groups of wild animals in the wild. It has been termed “the Self-Organizing Migrating Algorithm” – or SOMA for short (for complete description, source codes etc. please see [5]).

SOMA, and generally speaking any evolutionary algorithm, can be used in regards to any optimization problem. Surprisingly, many problems can be defined as optimization problems, e.g. the optimal trajectory of robot arms; the optimal thickness of steel in pressure vessels; the optimal set of parameters for controllers; optimal relations or fuzzy sets in fuzzy models; and so on. Solutions to such problems are usually more or less hard to arrive at, their parameters usually including variables of different types, such as real or integer variables. Evolutionary algorithms are quite popular because they allow the solution of almost any problem in a simplified manner, because

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they are able to handle optimizing tasks with mixed variables - including the appropriate constraints, as and when required.

This contribution explains SOMA's use on static optimization of given chemical reactor. A large part of the research dealing with wastes of the leather industry, except for USDA publications, does not go into particulars about how to cope with chrome sludge after dechromation of tanned wastes. As if chrome sludge so formed was automatically assumed to be simply used for producing recycled tanning salt. Even though the balance of chromium in chrome-tanned wastes and of necessary tanning salt is very favorable for recycling in the tanning industry, the actual situation is different.

Although we quite correctly feel and hope that the issue of recycling chromium into the tanning industry should be worked on or at least supported by manufacturers of chromic chemicals in the first place, we studied both the drawbacks of such recycling and applications in other fields. Part of this research is focused on reactor inside which class of mentioned chemical reactions could be done. Main aim of SOMA use was for reactor static optimization.

2 Reactor Description

Model of the reactor (see Figure 1) inside which can be realized above mentioned reactions was given by 5 nonlinear partial differential equations. Expert parameters were used for original setting. They comes from experiences obtained during visit in laboratory „Resine and Composite for Forest Products" in Sainte-Foy, Canada. This set of parameters consisted of two kind of parameters i.e. parameters of chemical materials and physical parameters of reactor under consideration. An initial conditions (a_{AP0}, a_{BP0}, a_{P0}, T_{P0}, T_{X0},) used in following simulations. This set of parameters was used for initial simulations. Both graphs show that reactor under expert parameters produce unsatisfactory behaviour. Reactor production stabilizes itself after 27 Hrs. on 15 % concentration of output chemical. From that point of view above-mentioned parameters were regarded like unsatisfactory. Because of these reasons a few static optimizations by SOMA algorithm were consequently done.

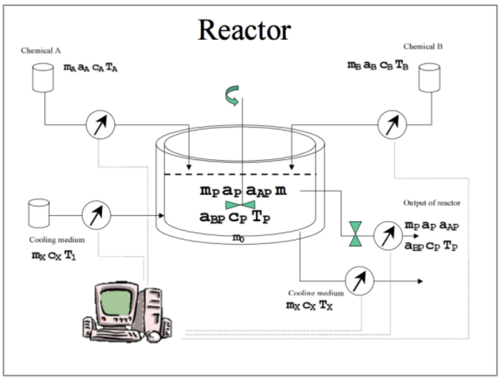
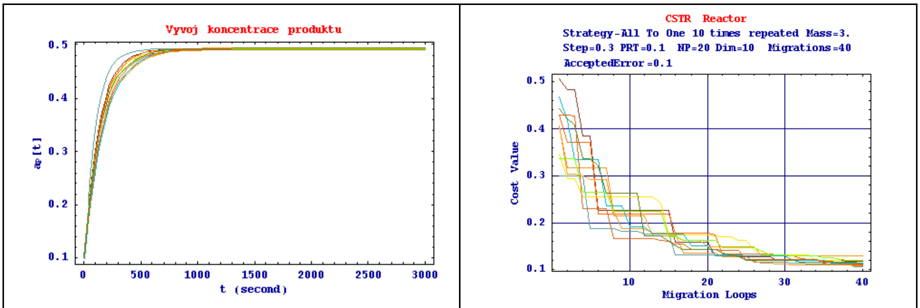


Fig. 1. Optimized reactor

They were done in following steps:

1. Optimization without restrictions - Fig. 2 a) and b)
2. Optimization with restrictions applied exactly in given time
3. Optimization with penalty applied during time interval
4. Optimization with penalty applied during time interval and sub optimization of cooling surface



a) mass fraction of a chemical product in the output stream

b) Cost value history in SOMA optimization

Fig. 2. a) reactor static optimization without penalty and restrictions, b) cost value history in SOMA optimization

The last static optimization is important one. The first three are mentioned here too only for complete overview, what optimizations were done by means of SOMA. Each of four optimization cases was 10 times repeated. From all 10 simulations was finally chosen the best reactor. According to this table a global extreme was found in 13-ti dimensional configuration space. Last 13th dimension was cost value of cost function. In case of the last optimization (optimization with penalty applied during time interval and sub-optimization of cooling surface) searching for global extreme had run in 11th dimensional space because of relations among some parameters.

3 Optimization without Restrictions

Main aim of this optimization was focused on parameter reactor optimizing in such way that a_{AP} =0.6 was desired. Others parameters like a_{BP}, a_{BP}, T_P, T_X was not restricted. The total number of simulation done here was 10. He maximum of a_{AP} was a_{AP} = 0.5, which can be regarded, like a good result. In all following simulations was not reached better result probably thanks to physical and chemical reasons. Despite this result a wrong behaviour can be observed on Fig. 2. One of no acceptable behaviour shows temperature that is very high (6000 K, -900 K, etc.). Such physical behaviour is not acceptable and also not realizable. Explanation of such wild behaviour stems from obvious fact that our model does not exactly follow reality. Cost function used in this simulation was given by

$$f_{\cos t} = \left|0.6 - a_P(t)\right| \quad where \quad t = 1200 \qquad (1)$$

Optimization was focused of such behaviour searching which should satisfy in time t = 1200 second minimal difference between desired value in this time and reactor output response in this time.

4 Optimization with Restrictions Applied Exactly in Given Time

In this simulation previous cost function was enlarged for set of operands. Difference between them was such that were penalized parameters a_{AP}, a_{BP}, a_P, T_P, T_X. It was expected that described cost function modification will delete unacceptable temperatures. Despite this fact some unacceptable temperatures were observed there, so this kind of optimization was still non-successful. These results were probably caused thanks to weak penalization applied only in time $\tau = 100$. Parameters a_{BP}, a_{BP} in are multiplied by 100 because of its support in final penalization. Without it parameters a_{BP}, a_{BP} would influent final cost function only a little bit because of its range a_{BP}, a_{BP} $\in [0, 1]$. Because this optimization still generated wrong solutions, following simulation was designed.

5 Optimization with Penalty Applied during Time Interval

In this simulation was minimized difference (surface) between desired and observed reactor response. It was expected from this simulation that high or low temperatures would not be observed here. Minimization of it should satisfy this. Parameters a_{BP}, a_{BP} in are multiplied by 100 because of the same reasons like in previous step. From results it is clear that this set of 10 simulations produce more reasonable behaviour than in previous cases. However, some error-behaviour is there too. For example a cooling medium temperature lower than 0 C_o can be observed there. This non-acceptable behaviour is probably caused by fact that between model and real reactor there is no 100% equivalency. Also some simplifications in computer model partly caused it.

For example physical relations between cooling surface and surface of reactor was not taken under consideration, etc. This was solved in the last and successful optimization.

6 Optimization with Penalty Applied during Time Interval and Suboptimization of Cooling Surface

This optimization was focused on optimal parameter searching in such way that some of these parameters were related among themselves. These parameters were m_A, m_B, m_P, m a S. Relation between m_A, m_B, a m_P was given by

$$m_P = m_A + m_B \tag{2}$$

This equation simply says that output is equal to sums of inputs. Next relation was between m a S (cooling only in the wall of reactor and on its bottom) and was described like

$$S = 2\pi r^2 + \pi r^2 \tag{3}$$

$$m = \varsigma \pi r^3 \quad where\ \varsigma = 1100\ kgm^{-3} \tag{4}$$

A simple presumption that "r" is equal to height "h" was done for simplification. Thus only "r" instead of "S" and "m" was used. Graphs based on 10 times repeated static optimizations are depicted on Fig. 6 a-d). There is visible that the best reactor produce not only reasonable behaviour (temperatures $T_P \approx 380$ K a $T_X \approx 340$ K) but also output chemical product $a_P = 0.5$ i.e. 50%, which represents quality increase for 35% ($a_{Poptimal} = a_{Poptimized} - a_{Pexpert} = 0.5 - 0.15 = 0.35$). Fact that this behavior is stabilized after 8-10 minutes (in comparison with **27 Hrs** (!!!) in case of expertly set reactor).

7 Conclusion

The methods of optimization mentioned here (detail at [5]) are relatively simple, easy to implement and easy to use. Despite that, it is capable of optimizing all integer, discrete and continuous variables and capable of handling non-linear objective functions with multiple non-trivial constraints.

A soft-constraint (penalty) approach is applied for the handling of constraint functions. Some optimization methods require a feasible initial solution as a starting point for a search. Preferably, this solution should be rather close to a global optimum to ensure convergence to it instead of a local optimum. If non-trivial constraints are imposed, it may be difficult or impossible to provide a feasible initial solution. The efficiency, effectiveness and robustness of many methods are often highly dependent on the quality of the starting point. The combination of the SOMA algorithm with the soft-constraint approach does not require any initial solution, but it can still take advantage of a high quality initial solution if one is available.

For example, this initial solution can be used for initialization of the population in order to establish an initial population that is biased towards a feasible region of the search space. If there are no feasible solutions in the search space, as is the case for totally conflicting constraints, SOMA algorithm with the soft-constraint approach are still able to find the nearest feasible solution. This is important in practical engineering optimization because often, many non-trivial constraints are involved. The approach described above was targeted to fill the gap in the field of mixed discrete-integer-continuous optimization, where no one single really satisfactory method appeared to be available. Despite being in its infancy, the described approach has great potential to become a widely used, multipurpose optimization tool for solving a broad range of practical engineering optimization problems.

These algorithms are undoubtedly one of the most promising and novel methods for non-linear optimization that can be applied generally, and they work with minimum assumptions with respect to the objective function.

The algorithm requires only the value of objective function for guidance of it's seeking the optimum. No derivatives or other auxiliary information are desired. Including the algorithm extensions discussed in this article, the SOMA algorithms can be applied to a wide range of optimization problems, which practitioners in the field of modern prediction would like to solve.

In the past, SOMA had been successfully used on hard optimization problems with good results (see [5]) During these tests, **9500** optimization simulations were carried out, which represent approximately **$22x10^6$** cost function evaluations. The quality of the results, and the fact that the conclusions derived from them could be proven to be true, have demonstrated that SOMA has the capability of finding optimal near-optimal solution with a very high reliability.

We have also mentioned the possibility of chemical reactor optimization by SOMA algorithm. Inside this reactor can be realized certain class of chemical reactions like enzymatic dechromation technology, etc. The advantage of the enzymatic reaction is the production of protein hydrolyzates of relatively good quality and chrome sludge. Using organic bases to form alkaline reaction mixture increases the quality of both is products. A partial regeneration of organic base when diluted protein hydrolyzates undergo concentration cuts the operating costs of enzymatic hydrolysis. In commercial application, the greatest volume of protein hydrolyzate is channeled into agriculture. Hydrolyzate, as an organic nitrogenous fertilizer, not only equals the combined ureaammonium nitrate fertilizer in crop yield, but also surpasses it manifolds in the foodstuff value of consumer's greens. The content of nitrates is as much as 200 times lower on average. Hydrolyzate is also used in the manufacture of biodegradable foil, especially for producing sowing tape. The main obstacle for the utilization of the chrome sludge is a relatively high content of proteins in the dry substance of cake. In closing, it may be said that enzymatic hydrolysis has a place in the treatment of chromium containing tannery waste and the funds expended on this field of research have brought satisfactory results.

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