Decision Engineering of an Decyl-lactose Generation Chemical Laboratory Process Assisted by a Diploid Genetic Algorithm and a Multicriterion Aggregation Method

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Abstract. In many, if not most, optimization problems, industrialists are often confronted with multiobjective decision problems. For example, in manufacturing processes, it may be necessary to optimize several criteria to take into account all the market constraints. So, the purpose is to choose the best tradeoffs among all the defined and conflicting objectives. In multicriteria optimization, after the decision maker has chosen all his objectives, he has to determine the multicriteria optimal zone by using the concept of domination criterion called the Pareto domination. Two points, in the research domain, are compared. If one is better for all attributes, it is a non dominating solution. All the non dominating points form the Pareto's region. In this paper, a multiobjective optimization algorithm is used to obtain this zone, based on a diploid genetic algorithm. This is compared to two industrial applications: food's granulation and decyllactose synthesis. In the optimal zone, the decision maker has to choose the best solution after he has made a ranking with all potential solutions. Finally, a Decision Support System shell is developed in order to classify all solutions.

1 INTRODUCTION

In a lot of domains, processing or product formulation depend on several objectives to take into account their different features. Extrusion processes for food are a good illustration for this case. For example, it may be necessary to optimize different parameters such as texture, flavour, and so on, in order to formulate a new product and to maximize yields, production and product quality with minimal investment whereas these criteria are not optimal for the same working conditions. In the engineering processes domain, multiple objectives have usually been combined, often through a linear combination, to form a scalar objective function [8] or a geometric average of these ones [17]. Another classical method consists in optimizing one chosen answer and in turning into constraints the others [14]. These techniques depend on the user's choice at the begining, so preferences can bias the results.

Methods incorporating a domination criterion are often more interesting because they are more general, more accurate and without *a priori* knowledge. The object is to find a non dominated zone in which a decision maker will be able to choose the best solution. This region, called the Pareto domain, is the set of all non dominated points. For the Pareto's domination criterion, a point dominats another if it is better for one criterion, and better or equal for the others. The aim of the study is not to find immediately the preferred solution but to exclude all conditions which are not interesting. This information allows to choose the industrial decision maker's preferences, because it restricts all possible choices, mistakes and bias.

Schaffer [15] describes an extension of the traditional Genetic Algorithm (GA) which allows the searching of the parameter space where multiple objectives are to be optimized. His VEGA (Vector Evaluated GA) gives a selection preference to the non dominated members of a population. But, only extreme points on the Pareto front seem to be found with VEGA, so Horn *et al.* [9] apply a niching pressure to spread its population out along the Pareto optimal tradeoff surface. Fonseca and Fleming [12], in the same way, use the non domination ranking for selection to move a population towards the Pareto front and a niching mechanism, such as sharing [13], to keep the GA from converging to a single point. Moreover, a direct intervention of an external Decision Maker (DM) gives interactive information in the multiobjective optimization loop. So, a satisfactory solution of the problem is found as soon as the knowledge is acquired [12].

In this study, the Pareto domain is obtained at first without external influences. The algorithm use an adapted GA, and is applied to several industrial. On the last step, the DM influences are taken into account and notions of decision engineering are required. So, the global multicriterion analysis leads to the best tradeoff.

2 THEORITICAL ALGORITHMIC BACKGROUND TO THE MULTIOBJECTIVE OPTIMIZATION

2.1 An improved Diploid Genetic Algorithm (DGA)

The multiobjective optimization methods developed use a DGA whose principles were elaborated by Perrin *et al.* [4].The diploid version is kept because its performances were found to be better compared with a haploid one [6]. Each individual (which can be a possible solution of the problem) is described by a four-tuple (a_j, a_j', D_j, x_j). a_j and a_j' represent the two alleles of the j gene, D_j is the dominance of one allele over the other chosen in {0,1} values and x_j represents the phenotype which is the result of the combination of the respective alleles, a_j and a_j' :

$$x_j = D_j.a_j + (1-D_j).a_j'$$

An initial population is created by generating a set of m points from the search area. Each point is tested and evaluated. If this population is not the solution, then genetic operators are used to make it evolve. Only the better individuals will survive (elitist selection) and participate in the creation of a new generation. The reproduction of the individuals in the diploid model consists of a multi-crossover of the two chromosomes of each parent, a mutation and a homozygosity. Mutation consists, for the selectionned individual, of a randomly draw for all the genes of the two chromosomes and all the dominances. Homozygosity allows to modify a child by copying the phenotype x of the two chromosomes a and a' ($x_j = a_j = a_j$'). All the genetic operators and their usefulness are detailed in [4]. If the generated child is worse than the worst parent, he is not adapted. He is eliminated and another is created. So dominance may be controlled to decrease the child death rate.

The dominance may be randomly chosen in {0,1} values. But, to keep dominance features, table 1 shows how to control D_j :

		Dominance of a_j in the first parent	
		Recessive	Dominant
Dominance of a_j' in The second parent	Recessive	Random	$D_j = 1$
	Dominant	$D_j = 0$	Function of the best parent

Table 1: *choice of the value of the dominance $D_j \in \{0,1\}$*

Statistically, children have more chances of being better than the parents with the control of the dominance, so the convergence of the algorithm speeds up and less points are tested.

The population of each generation is evaluated until it satisfies the stop criterion: $f_{max} - f_{min} < \varepsilon$ where f_{min} and f_{max} are respectively the minimal and the maximal objective function values in the current population and ε is the given precision for solution estimation.

2.2 Use of one function to define the set Pareto

Previously, a multicriteria optimization algorithm was elaborated by Viennet *et al.* [7], but it need three steps, and the number of points in the Pareto set was not controlled. The aim of this section is to define one function to make a monocriteria optimization with the DGA. A set of m given points is randomly generated. All individuals are evaluated by the calculation of each objective f_i (i = 1,…n). Then, for each point x_j, a value is associated, $F(x_j)$, the number of times that it is dominated by all the others in the current generation:

$$F(x_j) = \sum_{p=1}^{m} h_{jp} \qquad \text{where } h_{jp} = 1 \text{ if } x_p \text{ dominate } x_j$$

$$h_{jp} = 0 \text{ else}$$

Let be denoted by n the number of criteria. For two points x_j and x_p in the same population, and for all criteria i (i = 1,..n):

if $f_i(x_j)$ WORSE THAN $f_i(x_p)$ $c_{ijp} = 0$
if $f_i(x_j)$ BETTER THAN $f_i(x_p)$ $c_{ijp} = n + 1$
if $f_i(x_j)$ EQUAL TO $f_i(x_p)$ $c_{ijp} = 1$

where c_{ijp} is an intermediate variable.
In the case of minimization WORSE THAN is equivalent to <, and BETTER THAN to >.

if $\sum_{i=1}^{n} c_{ijp} < n$ then $h_{jp} = 1$ and $h_{pj} = 0$ because x_j is dominated by x_p.

if $\sum_{i=1}^{n} c_{ijp} \geq n$ and $\sum_{i=1}^{n} c_{ipj} \geq n$ then $h_{jp} = h_{pj} = 0$ ($h_{jj} = 0$).

So, for each point, a value F corresponds by applying the Pareto's domination criterion. Then, all the points may be classified. The value of the function for the better individuals in the current generation is equal to zero. The classified individuals and their function value are presented in Table 2 in the k^{th} generation:

X	x_1	x_2	x_3	....	x_s	x_{s+1}	....	x_t	x_{t+1}	....	x_m
F	0	0	0	....	0	$F(x_{s+1})$	....	$F(x_t)$	$F(x_{t+1})$	....	$F(x_m)$

Table 2: *classified individuals in the k^{th} generation*

The s better individuals are non dominated in the current population (k) and are the chosen parents for the next (k+1). The (m-s) worse individuals are eliminated for the next generation but are used for the children evaluation. Each new individual is compared with all m points in the previous population. Then, a threshold t is defined to keep the better children:

$t = s + E[0.3*(m-s)]$ where E[x] is the entire part of x
and 0.3 is empirically choosen

So, a child death rate is applied to the convergence when the new individual x_j is worse than the x_t point, *i.e.* $F(x_j) > F(x_t)$. When the new population is reformed, all the m points are evaluated with the new values of the function F. The population of each generation is evaluated until the stop criterion is satisfied: all the points are non dominated, that is to say that F is equal to zero for the m points.

The DGA is used only once and the algorithm converges rather rapidly (3 to 5 generations, depending on the problem). The most interesting thing is that the number of points in the Pareto's zone is controlled whatever the sproblem studied. If 5000 points are required to clearly draw the Pareto's area, it is represented by all these points with a lot of accuracy and without an increasing calculus time.

3 PARETO DOMAIN DETERMINATIONS

3.1 Extrusion process

Food granulation for cattle is presented as an industrial application. The goal is the optimization of the working conditions of an extrusion process described by Courcoux *et al*. [8]. A pulverulent product is converted into granules due to the conjugated effects of heat, moisture and pressure. The industrialist would like to simultaneously minimize moisture and friability of his product and the energetic consumption of the process. For modelling these criteria, an experimental design is realised [8]. Factors having an influence on this process are the feeding rate, speed of rotation for mixing, flour temperature, speed of rotation and drawplate profile. For this study, only two factors are taken into account, the flour temperature T, situated between 35 and 75 °C, and the drawplate profile D, between 2 and 6 cm (figure 2).

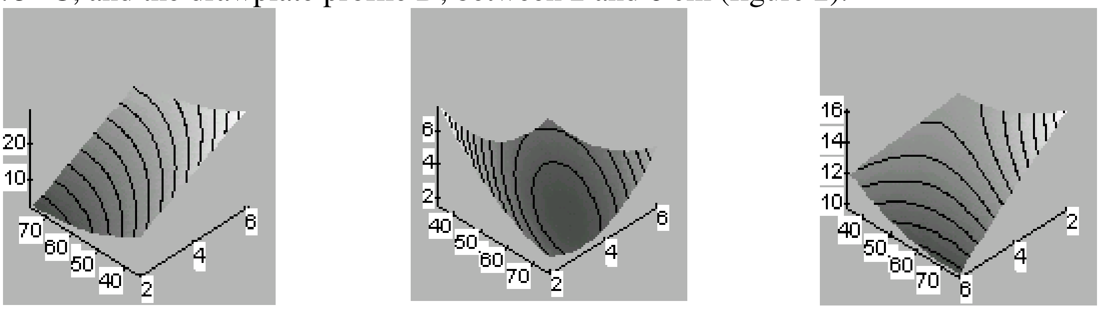

Figure 2: *The evolutions of energetic consumption, friability index and moisture of granules vs the temperature and drawplate profile, by Courcoux et al. [8]*

The optimal Pareto's zone, obtained by our algoritm, is represented in figure 3 by black points.

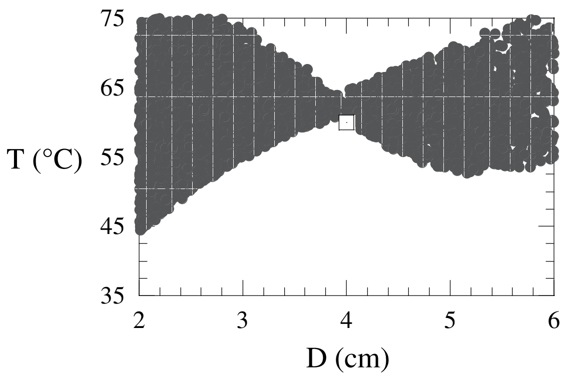

Figure 3: *representation of the optimal Pareto's for the example of an extrusion process*

The method give satisfactory results for the Pareto's zone, and keeps 5000 points for its representation. It allows to have a precise area with a controlled number of points. So, the decision maker will be able to choose in this zone the best point.

3.2 Decylaction of lactose synthesis

The technique for Pareto region determination is applied to the definition of an optimal working zone for the synthesis of a biosurfactant derived from lactose: the decyllactose. For this study, 3 factors are considered, lactose concentration between 10 and 320 g/l, sodium hydride/lactose molar ratio between 1 and 8 and decyliodide/lactose molar ratio between 1 and 4. Three responses are maximized: reaction yield (decyllactose produced/initial lactose concentration), lactose conversion rate and productivity (decyllactose produced/time of reaction). A fourth one is minimized: biosurfactant cost price. This reaction is carried out during 3 hours at 35°C.

In figure, triangles show positions of experiments obtained from Fuzzy Dynamic Experiment Design, a technic developped in our laboratory. The banned and undefined zones correspond to experimental conditions where product formation is impossible or improbable due to physico-chemical conditions. Radial Basis Functions neural networks are used for modelling each response.

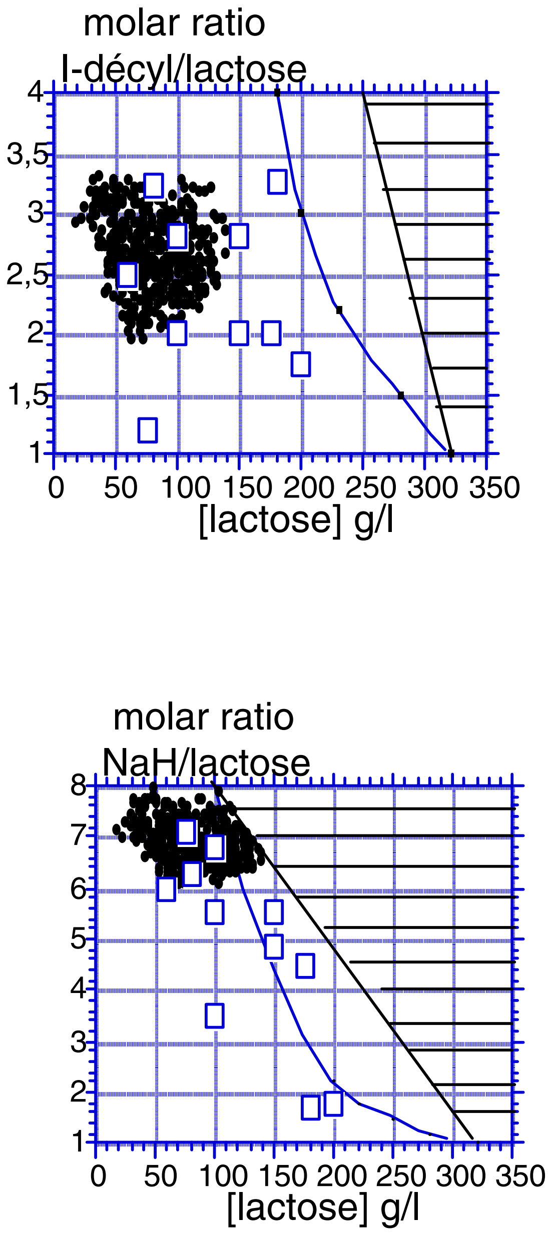

Figure 6 : *Pareto set and experiments performed.*

4 MULTICRITERION ANALYSIS FRAMEWORK

4.1 An original approach

Many real problems can be modeled as multicriterion problems but the decision engeneering knowledge intervention in a specific chemical engineering competence field as the cattle-food granulation process is a very interesting new research. We dare to believe that even if our results are inscribed in a relatively narrow axis and in spite of their limits, they will contribute to the development of the knowledge in the chemical process engineering and in the decision making sciences.

This process control problem can obviously be most appropriately structured around an ELECTRE type **o**utranking **s**ynthesis **a**pproach (OSA) [11]. The main reasons justifying our choice are, in fact, the realistic way in which this OSA links the preferences; this is somewhat similar to the "democratic" principle much more natural when faced with a decision having product quality and product profitability impacts.

4.2 Algorithmic design

Let us consider the *input parameters' set of the granulation process* containing the discretized *temperature* (between 35 and 75 C^{o}) and *drawplate profile* D (between 2 and 6 cm) values on the one hand and *the output parameters'set of the granulation process* containing three criteria, namely the energetic consumption, the friability index and the moisture of the granules on the other hand. The criteria role has been attributed to the output parameters'set of the granulation process, i.e. *energetic consumption*, *friability index* and *moisture of granules* (to minimize the 3), even when the alternatives role has been attributed to the input parameters'set of the granulation process, *i.e. temperature* and *drawplate profile*.

Our multicriterion analysis algorithm is essentially a comparison process where the decision maker's preferences are expressed by means of some constraint-like parameters: indifference, preference, veto thresholds and the weights of the criteria. In order to operationally run the **m**ulticriterion **a**nalysis **p**rocess (MAP), it is necessary to introduce the MAP's input set Ψ with the following synoptic structure [3]:

$$\Psi = \Gamma_{\S}\ [m, n, M_{[m\times n]}, K_{[n]}, \Phi_{[n]}, R_{[n]}, Q_{[n]}, P_{[n]}, V_{[n]}, W_{[n]}]$$

where

- $\Gamma_{\S}$ - MAP's algorithm;
- m - number of alternatives;
- n - number of criteria;
- $M_{[m\times n]}$ - real m x n cardinal matrix containing the alternatives'evaluations in relation to the criteria and $\overline{m}_{ij} = f_j(x_i) \in M_{[m\times n]}$; i = 1,…,m; j = 1,…,n;
- $K_{[n]}$ - binary n cardinal vector indicating the nature of the criteria evaluation, with

$$\kappa_j = \begin{cases} 0 & \text{if the evaluation in relation to the } j^{th} \text{ criterion is an ordinal type} \\ 1 & \text{if the evaluation in relation to the } j^{th} \text{ criterion is a cardinal type} \end{cases}$$

and $\kappa_j \in K_{[n]}$; j = 1,…,n (in this paper all the criteria are cardinal type);

- $\Phi_{[n]}$ - binary n cardinal vector indicating the nature of the orientation of the criteria, with

$$\phi_j = \begin{cases} 0 & \text{if the } j^{th} \text{ criterion is to be minimized} \\ 1 & \text{if the } j^{th} \text{ criterion is to be maximized} \end{cases}$$

and $\phi_j \in \Phi_{[n]}$; j = 1,…,n (0 for all criteria in this paper);

- $R_{[n]}$ - real n cardinal vector containing the range for every criteria

and $\rho_j \in R_{[n]}$; j = 1,…,n;

- $Q_{[n]}$ - real n cardinal vector containing the indifference thresholds and $q_j \in Q_{[n]}$; j = 1,…,n;

- $P_{[n]}$ - real n cardinal vector containing the preference thresholds

and $p_j \in P_{[n]}$; j = 1,…,n;

- $V_{[n]}$ - real n cardinal vector containing the veto thresholds

and $v_j \in V_{[n]}$; j = 1,…,n;

- $W_{[n]}$ - real n cardinal vector containing the criteria's relative importance coefficients w_j

and $w_j \in W_{[n]}$; j = 1,…,n.

The following relations must be verified between the thresholds:

$$0 \le q_j \le p_j \le v_j \le \rho_j; \; j = 1,\ldots,n$$

The relative importance coefficients are normalized, i.e. $\sum_{j=1}^{n} w_j = 1$.

This input set Ψ is processed using the MAP algorithm $\Gamma_{\S}$ to determine the ranking from the best to the worst (i.e. *"nadir"*) alternative with possible *ex aequo.*

$C\|[i;\bar{i}]$ is calculated as follows:

$$C\|[i;\bar{i}] = \sum_{j=1}^{n} w_j \cdot \delta_j\|[i,\bar{i}]; \; i = 1,\ldots,m; \; \bar{i} = 1,\ldots,m; \; i \ne \bar{i}; \; j = 1,\ldots,n.$$

where $\delta_j\|[i,\bar{i}] = \begin{cases} 1 & \text{if } -\Delta_j \le q_j \\ \dfrac{\Delta_j + p_j}{p_j - q_j} & \text{if } q_j < -\Delta_j \le p_j \\ 0 & \text{if } p_j < -\Delta_j \end{cases}$

and $\Delta_j = \overline{m}_{ji} - \overline{m}_{j\bar{i}} \in M_{[m \times n]}$; j = 1,…,n; i = 1,…,m; $\bar{i}$ =1,…,m; $i \ne \bar{i}$. If some criteria call for maximization while others require minimization, we have introduced two temporary *sentries* (i.e. guards) variables k and $\bar{k}$ in our calculations of Δ_j.

If $\phi_j = 0$, meaning that this criterion is to be minimized, then $k = \bar{i}$ and $\bar{k} = i$, else if $\phi_j = 1$ (criterion to be maximize) k = i and $\bar{k} = \bar{i}$; this way $\Delta_j\|[i,\bar{i}] \equiv \Delta_j = \overline{m}_{jk} - \overline{m}_{j\bar{k}}$; $\forall \phi_j$; j = 1,…,n; k = 1,…,m; $\bar{k}$ = 1,…,m; $k \ne \bar{k}$.

A discordance index $\mathbf{D}_j\|[i;\bar{i}]$ is also calculated for every pair of alternatives at each criterion level as with ELECTRE III:

$$\mathbf{D}_j\|[i;\bar{i}] = \begin{cases} 0 & \text{if } -\Delta_j \le p_j \\ \dfrac{-\Delta_j - p_j}{v_j - p_j} & \text{if } q_j < -\Delta_j \le v_j \\ 1 & \text{if } v_j < -\Delta_j \end{cases} ; j=1,\ldots,n, i=1,\ldots,m, =1,\ldots,m, \; \bar{i}=1,\ldots,m; i \ne \bar{i} \; .$$

Using the concordance and discordance indexes, we generate outranking degrees $\sigma\|[i;\bar{i}]$ for every pair of alternatives. These outranking degrees are obtained using the following Rousseau-Martel formula: $\sigma\|[i;\bar{i}] = C\|[i;\bar{i}] \prod_{j=1}^{n} \left[1 - \left(\mathbf{D}_j\|[i;\bar{i}]\right)^3\right]$; i = 1,…,m; $\bar{i}$ =1,…,m; $i \ne \bar{i}$ [10].

The obtained outranking relation sets may be represented as an outranking matrix. Working with outranking relations implies synthetizing that matrix in such a way as to provide a process control recommendation in the form of an alternative ranking.

We make that synthesis following the notion of *outgoing flow* and *incoming flow* from PROMETHEE [16].
For calculations we use:

$$\sigma_i^+ = \begin{cases} \sum_{i=1}^{m} \sigma\left\|[i;\bar{i}]\right. & \text{if } i \neq \bar{i} \\ 1 & \text{if } i = \bar{i} \end{cases} \quad \text{and} \quad \sigma_i^- = \begin{cases} \sum_{i=1}^{m} \sigma\left\|[\bar{i};i]\right. & \text{if } i \neq \bar{i} \\ 1 & \text{if } i = \bar{i} \end{cases} ;\ i = 1,\ldots,m;\ \bar{i} = 1,\ldots,m;\ i \neq \bar{i}$$

and we get the total ranking of the alternatives from the *net flow* as in PROMETHEE II:

$$\sigma_i = \sigma_i^+ - \sigma_i^- \quad i = 1,\ldots,m.$$

4.3 Results

4.3.1 Extrusion

In order to illustrate the proposed treatment, firstly we present the results of the extrusion process, using the earlier described $\Gamma_{\S}$ algorithm. We have developed a Decision Support System (DSS) shell based on our multicriterion analysis conception with the tresholds indicate in table 3.

	q_j	p_j	v_j
Friability index	0.2	0.5	0.8
Moisture	0.5	1.5	3
Energetic consumption	1	3	6

Table 3: *indifference, preference and veto tresholds for each criterion*

Table 4 gives the best and the worst alternatives in the Pareto domain, after the total ranking has been made:

Best		**Nadir**	
D (cm)	T (°C)	D (cm)	T (°C)
3.3186	64.909	5.2921	72.677

Table 4: *best and worst parameters alternatives*

This DSS shell produces very encouraging final results as process control recommandation for the chemical engineering. To illustrate the robustness of the results, we present *quintile* by *quintile* the input parameters of the granulation process as well as the positions of the best and the worst input parameters (Figure 5). Each *quintile* contains 20% of the points in the Pareto set.

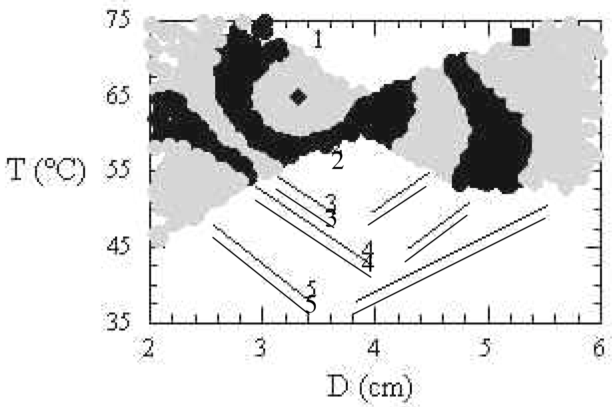

Figure 5: *Best (◆) and worst (■) conditions giving by DSS shell*

We can notice that the best point is a robust one and the little variations of the working conditions do not alter much the product quality, the point stay in the Pareto domain. On the contrary, the worst point is on the borderline of the zone and so is not robust. The *quintiles* are represented by concentric zones (first zone: ●, second zone: ●, third zone: ●, *etc*…).

4.3.2 Decylactation of lactose

Secondly we present the results concerning the decylactation of lactos process, using the same $\Gamma_{\S}$ algorithm, but with the readjusted indifference, preference and veto tresholds for each criterion applied in the decylactation of lactose context.
Table 5 gives the best and the worst alternatives in the Pareto domain, after the total ranking has been made:

Best		**Nadir**	
Lactose (g/l)	Molar ratio NaH/lactose	lactose (g/l)	Molar ratio NaH/lactose
97.889261	6.334321	115.52411	7.233606

Table 5: *best and worst parameters alternatives for the decylactation of lactose process*

The following figure illustrate the very encouraging robustness of the results, by presenting the input parameters of the decylactation of lactose process as well as the positions of the best and the worst input parameters (Figure 6).

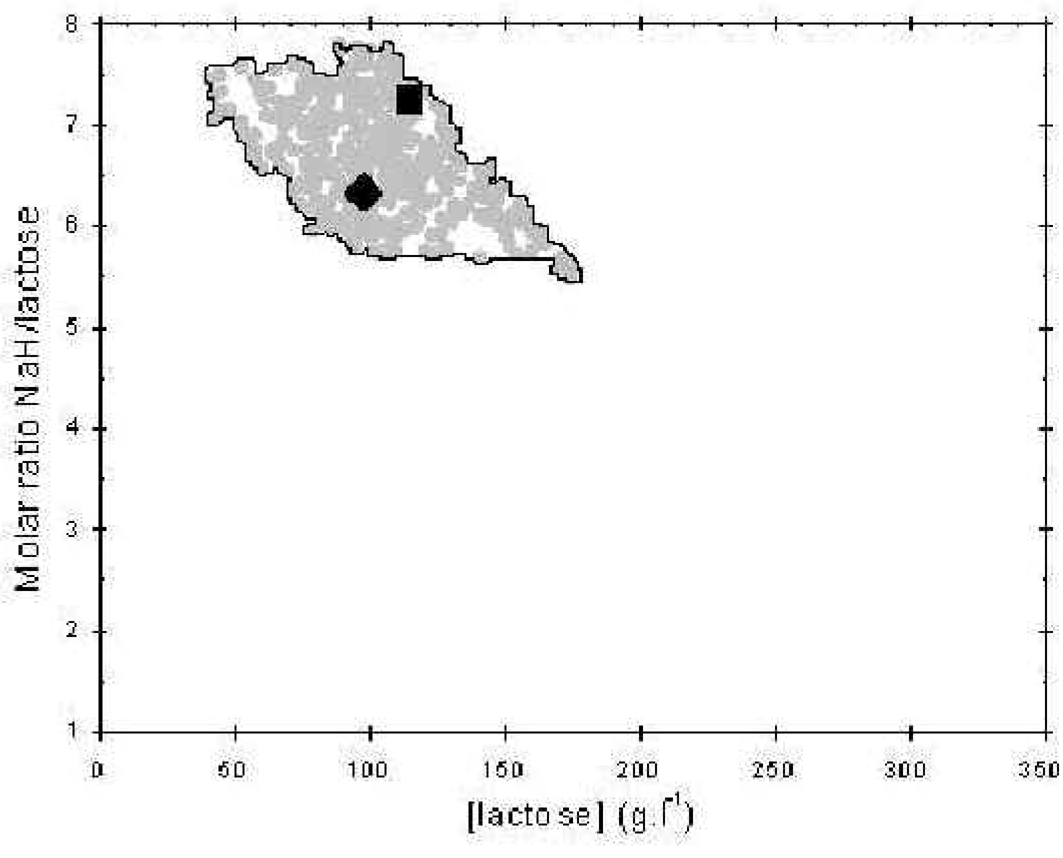

Figure 6: *Best (◆) and worst (■) conditions giving by DSS shell*

5 CONCLUDING REMARKS AND FURTHER CONSIDERATIONS

In this paper, a multiobjective decision problem is treated in order to explain an extrusion process and an decyl-lactose generation chemical laboratory process The main objective is the determination of the discussed chemical process's operating conditions which correspond not only to the traditional optimization problems, but also to the choice of the operating conditions according to the desired technological, chemical engineering priorities or preferences of the decision maker. So, the proposed steps (at first, the determination of the multiobjective optimal zone and then the multicriterion analysis) give a lot of data to choose the best tradeoff of the problem.This type of analysis design concerns principally the decisional engineering competence, but requires also a good knowledge of the chemical phenomena as well as the definition of a sufficiently precise model.

In order to respect the paper length constraint, we precise that our summerizing remarks regarde first of alls the granulation process, although one could formulate semantically similar remarks also relating to the decylactation of lactose process.

Our DSS shell gives the complete ranking of the Pareto domain. We notice the robustness of the best operating conditions, *i.e.* it can stay in the same *quintile* even with small variations of temperature and profile drawplate. It is an important result for the decision making science.

The results of our analysis can be registered in the chapter of the innovating contributions of the art of chemical engineering and opens promising perspectives towards the exploration for the decision robustness problem concerning the effective control of the chemical processes. For example, one of the close perspectives is to apply the analysis to polymerization processes which are more complex for modelling [2]. On the other hand, decision engineering applied to chemical engineering leads us to define decision parameters (w_j, p_j, q_j, v_j, $\forall$ j) in the form of intervals or with fuzzy membership functions. In the case of a complex process, the natural difficulty to define simple preferences leads to adapt decision engineering techniques. The objective is to search for the decision capable of staying the best (or among the best) in spite of small parameter variations. So, adaptation techniques and new projections in the decision aid science will be needed to solve the problem of decision robustness.

It seems that our paper proves even the natural *raison d'être* of the symbiosis between scientific disciplines apparently very different, such as the science of decision making and the chemical science in the area of controling various processes. Now, chemical engineering has the possibility to solve its multiobjective decision problems and decision engineering can adapt their techniques to chemical industrial problems.

We hope by conviction that this present process control related research constitute a first step towards the axiomatization of the multicriterion control of the real time decision-making processes, whose industrial application is promising and innovative.

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